Heat Equation

Heat equation governs the temperature distribution in an object. According to the second law of thermodynamics, if two identical bodies are brought into thermal contact and one is hotter than the other, then heat must flow from hotter body to the colder one at a rate proportional to the temperature difference of the two bodies. Therefore, in a metal rod with non-uniform temperature, heat (thermal energy) is transferred from regions of higher temperature to regions of lower temperature. Consider a uniform rod of length L with non-uniform temperature lying on the x-axis from x = 0 to x = L. Assume that the lateral surface of the rod is perfectly insulated, and heat can enter or leave the rod through either of the rod ends and thereby creating a 1D temperature distribution.

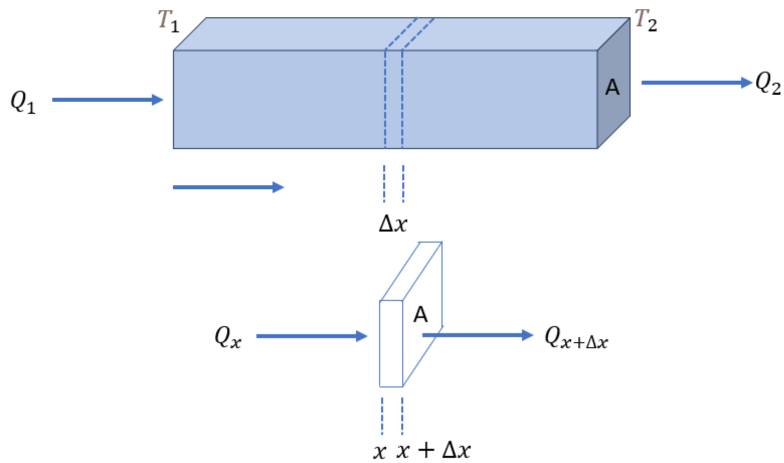


Fig. 1: A rectangular metallic rod with insulated lateral surface and nonuniform heat distribution along length.

Consider an arbitrary thin slice of the rod of width Δx, between x and x+ Δx. The slice is so thin that the temperature throughout the slice is T (x, t). The time heat energy needs to transit through the tiny slice is Δt. The Heat (or thermal) energy of a body with uniform properties is defined as:

$$Q(x,t) = c \times m \times T = c(x) \times \rho(x) A\Delta x \times T(x,t) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

Where, c(x) is the specific heat of the material, defined as the amount of heat energy that it takes to raise one unit of mass of the material by one unit of temperature [$c(x) > 0$]. The specific heat may not be uniform throughout the bar and in practice the specific heat depends upon the temperature. However, this will generally only be an issue for large temperature differences. T(x, t) is body temperature at any point x and any time t, m is the body mass. ρ(x) is the mass density which is the mass per unit volume of the material. The mass density may not be uniform throughout the rod.

Let $S(x,t)$ be the heat energy generated per unit volume at location x, and time t. Then, the total energy generated inside the thin slice is given by:

$$\Delta Q_g = A \times \Delta x \times S(x,t) \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Now let, Φ (x, t) be the heat flux that is the amount of thermal energy that flows to the right per unit surface area per unit time. The "flows to the right" bit simply tell us that if ϕ (*x*, *t)* > 0 for some *x* and *t* then the heat is flowing to the right at that point and time. Likewise, if ϕ (*x*, *t*) < 0 then the heat will be flowing to the left at that point and time.

According to the law of conservation of energy, the time rate of change of the heat stored at a point on the rod is equal to the net flow of heat into that point.

Change of heat energy of the segment in time Δt	+	Total heat energy generated inside the segment	=	Heat in from left boundary	-	Heat out from right boundary

$$c(x)\ \rho(x)\ A\ \Delta x[T(x,t+\Delta t) - T(x,t)] + A\ \Delta x\ S(x,t)\ \Delta t$$
$$= A\ \Delta t\ \varphi(x,t) - A\ \Delta t\ \varphi(x+\Delta x,t)\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (3)$$

Dividing both sides by $A\ \Delta x\ \Delta t$, equation (3) becomes:

$$c(x)\ \rho(x)[\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t}] + S(x,t) = \left[\frac{\varphi(x,t)-\varphi(x+\Delta x,t)}{\Delta x}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (4)$$

The above equation contains two unknown functions T and φ, both of which are function of both time and space. According to Fourier's law of heat transfer, rate of heat transfer is proportional to negative temperature gradient.

$$\varphi(x,t) = -k(x)\frac{\boldsymbol{\partial T}}{\boldsymbol{\partial x}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

Where $k(x)$ is the thermal conductivity of the material being studied and measures the ability of the material to conduct heat energy. Thermal conductivity can vary with the location of the rod as well as the temperature. But for small change in total temperature (less than 10 degree), the thermal conductivity can be treated as temperature independent. Now applying Fourier law and then rearranging equation (4) we have,

$$c(x)\rho(x)\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} = k(x)\left[\frac{\left(\frac{\partial T}{\partial x}\right)_{x+\Delta x} - \left(\frac{\partial T}{\partial x}\right)_x}{\Delta x}\right] + S(x,t) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Now taking the limit Δt, Δx → 0 equation (6) becomes:

$$c(x)\rho(x)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}[k(x)\frac{\partial T}{\partial x}]\ + S(x,t)\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (7)$$

Now assume that the material in the rod is uniform in nature and thus the thermal properties (specific heat and thermal conductivity) and mass density all are constants.

$$c(x) = c;\ \rho(x) = \rho; and\ k(x) = k$$

The heat equation then takes the form:

$$c\rho \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + S(x,t) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (8)$$

The above equation can further be simplified by defining the thermophysical term: thermal diffusivity to be

$$\alpha = \frac{k}{c\rho}$$

The heat equation then takes the form:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{S(x,t)}{c\rho} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (9)$$

This is 1D form of heat equation. We can get the 2D and 3D version of heat equation by using Laplacian operator to the first term in right hand side of equation (9)

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{S(x,t)}{c\rho} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (10)$$

Tow-Temperature Model

The Two Temperature Model (TTM) or Parabolic Two Step (PTS) model is given by:

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial x}\left(K_e(T_e, T_l) \frac{\partial T_e}{\partial x}\right) - g(T_e - T_l) + S(x,t) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (10)$$

$$C_l \frac{\partial T_l}{\partial t} = g(T_e - T_l) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (11)$$

Where,

C_e	:	Heat capacity of electrons
C_l	:	Heat capacity of lattice
g	:	Electron-phonon coupling factor
K_e	:	Thermal conductivity
$S(x,t)$	:	Laser source term, heat energy generated per unit volume per unit time.

The electron-phonon coupling factor and the lattice heat capacity are assumed to be constant. The electron heat capacity is a strong function of the electron temperature and thermal conductivity is obtained from electron and lattice temperature and equilibrium electron thermal conductivity measured at room temperature.

$$C_e = C_e^{\prime} T_e \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (12)$$

$$K_e(T_e, T_l) = k \frac{T_e}{T_l} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. (13)$$

Where, k is the equilibrium electron thermal conductivity measured at room temperature. The laser source term has an exponential decay in space to account for absorption in a nontransparent media, and a Gaussian shape in time. Neglecting the temperature dependence of the optical properties a reasonable approximation of the source term is given as.

$$S(x,t) = (1-R)\frac{J}{t_p d} * \exp\left[-\frac{x}{d} - 2.77\left(\frac{t}{t_p}\right)^2\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(14)$$

Where,

R	:	Reflectivity of the material
J	:	Laser fluence
d	:	Radiation penetration depth
t_p	:	Pulse width

Here R and α are material properties and J and t_p are laser parameters.

Solution of 1D Heat Equation

According to the law of thermodynamics, the system must undergo a process that brings the metal rod into thermal equilibrium irrespective to the initial temperature distribution of the rod. The way in which it proceeds to the thermal equilibrium is uniquely specified by the initial and boundary conditions. Therefore, the temperature distribution of the body depends on three factors: (i) the heat equation, which governs the rules for transferring thermal energy from one point to another within the body, (ii) the initial condition, which defines the initial temperature distribution of the body and (iii) the boundary conditions, which describe the effects of temperature and/or heat flux at the boundaries of the metallic rod. The heat equation involves a first order time derivative and a second order spatial derivative. The first order time derivative indicates that, the solution needs one initial condition, and the second order spatial derivative indicates that, the solution needs two boundary conditions.

The initial condition is the initial temperature which is constant for uniform metallic rod and usually set to the room temperature (300 K) is given

$$T(x,0) = T_0(x) = T_0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

Boundary conditions specified the temperature and/or heat flux at both ends of the metal rod. The most common boundary conditions are described below:

i. **Dirichlet Conditions:** These are also called prescribed temperature boundary conditions. The inhomogeneous Dirichlet conditions are given by
$T(0,t) = T_L(t);\ T(L,t) = T_R(t) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. 12.1.a$

If the temperature on both ends of the metal rod are constant and equal, then the boundary conditions are called homogeneous Dirichlet conditions and is given by:

$T(0,t) = T(L,t) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. 12.1.b$

ii. **Neumann Conditions:** These conditions are also called prescribed heat flux conditions and are given by:

$$-k(0)\frac{\partial T}{\partial x}(0,t) = \varphi_L(t); \quad -k(L)\frac{\partial T}{\partial x}(L,t) = \varphi_R(t) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 12.2.a$$

If either of the boundaries are perfectly insulated, then there is no heat flow out of them. Then Neumann Boundary condition is then referred to as the thermal-insulation boundary conditions and is given by:

$$\frac{\partial T}{\partial x}(0,t) = \frac{\partial T}{\partial x}(L,t) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 12.2.a$$

iii. **Robins Conditions:** These boundary conditions usually used when the metallic rod is in a moving fluid and utilize Newton's law of cooling. Robins conditions are described by the following equations:

$$-k(0)\frac{\partial T}{\partial x}(0,t) = H[T(0,t) - g_L(t)]; \quad -k(L)\frac{\partial T}{\partial x}(L,t) = H[T(L,t) - g_R(t)] \ldots\ldots\ldots 12.3$$

Where, H is a positive quantity that can be experimentally determined $g_L(t)$ and $g_R(t)$ give the temperature of the surrounding fluid at the two boundaries.

iv. Periodic Boundary Conditions: Periodic boundary conditions are used when a system of equations has to solve in infinite domain and can be given for the metallic rod studied here by:

$$T(-L,t) = T(L,t); \quad \frac{\partial T}{\partial x}(-L,t) = \frac{\partial T}{\partial x}(L,t) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (12.4)$$

In this study the homogenous Dirichlet boundary condition will be used to solve the heat equation without including source term and thermally insulated Neumann conditions will be used for solving 1D heat equation with a source term involved. Both analytical and numerical solution will be attempted.

Analytical Solution of 1D heat Equation for Two Temperature Model (TTM) using Thermal-insulation Boundary Condition

The assumptions made during analytical solution of heat equations are: laser source term is instantaneous and the thermophysical properties are constant. The PDEs are nonlinear due to the strong temperature dependence of electron heat capacity and thermal conductivity. The assumption of constant thermophysical properties makes the equations linear. For low level of laser fluence and laser pulse duration less than thermalization time this solution provides a very good approximation of experimental TDTR scan and brings up the nonequilibrium effects of laser heating when the electron and lattice systems reached in thermal equilibrium. This solution cannot resemble electron temperature properly as the temperature dependence of electron heat capacity is ignored.

Assuming constant thermophysical properties equations 10 and 11 can be combined and eliminated the electron temperature.

$$(C_e + C_l)\frac{\partial T_l}{\partial t} + \frac{C_e C_l}{g}\frac{\partial^2 T_l}{\partial t^2} = k\frac{\partial^2 T_l}{\partial x^2} + \frac{C_l}{g}k\frac{\partial^2}{\partial x^2}\left(\frac{\partial T_l}{\partial t}\right) + S(x,t)$$

$$C\frac{\partial T_l}{\partial t} + v\frac{\partial^2 T_l}{\partial t^2} = k\frac{\partial^2 T_l}{\partial x^2} + \mu k\frac{\partial^2}{\partial x^2}\left(\frac{\partial T_l}{\partial t}\right) + S(x,t) \dots\dots\dots\dots\dots\dots\dots (15)$$

Where, $C = C_e + C_l; v = \frac{C_e C_l}{g}; and\ \mu = \frac{C_l}{g}$

Applying the law of energy conservation, the laser source term can be rewritten by integrating the Gaussian source term over time and multiplied by delta function.

$$S = (1-R)\frac{J}{d}\exp\left(-\frac{x}{d}\right)\delta(t) \dots\dots\dots\dots\dots\dots\dots (16)$$

The deposition of energy from the laser source and absorption by electrons are instantaneous events. Therefore, the electron temperature distribution can be obtained by neglecting the diffusion and electron-phonon coupling term from equation 10.

$$C_e\frac{\partial T_e}{\partial t} = S$$

The electron temperature distribution then can be achieved by integrating the equation just after arrival of the heating pulse.

$$\int_{0^-}^{0^+} C_e\frac{\partial T_e}{\partial t}dt = \int_{0^-}^{0^+} S\, dt$$

$$\int_{0^-}^{0^+} C_e \frac{\partial T_e}{\partial t} dt = \int_{0^-}^{0^+} (1-R)\frac{J}{d}\exp\left(-\frac{x}{d}\right)\delta(t)\, dt$$

$$T_e(x, 0^+) = \frac{(1-R)J}{dC_e}\exp\left(-\frac{x}{d}\right) \ldots\ldots\ldots (17)$$

The initial condition is the initial temperature which is set to the room temperature. For simplicity we can assume the initial lattice temperature is zero and the first initial condition is given by.

$$T_l(x, 0^+) = T_l(x, 0^-) = 0 \ldots\ldots\ldots (18a)$$

From equation 11 we have

$$C_l \frac{\partial T_l(x, 0^+)}{\partial t} = gT_e(x, 0^+)$$

The second initial condition can be found by substituting for $T_e(x, 0^+)$ from equation 17.

$$\frac{\partial T_l}{\partial t}(x, 0^+) = \frac{g(1-R)J}{dC_eC_l}\exp\left(-\frac{x}{d}\right)$$

$$\frac{\partial T_l}{\partial t}(x, 0^+) = \frac{(1-R)J}{vd}\exp\left(-\frac{x}{d}\right) \ldots\ldots\ldots (18b)$$

During the short period of laser heating, heat losses from the front and back surfaces of the film can be neglected, leading to the thermal-insulation boundary conditions:

$$\frac{\partial T_l}{\partial x}(0, \quad t) = \frac{\partial T_l}{\partial x}(L, \quad t) = 0 \ldots\ldots\ldots (19)$$

Where L is the film thickness. The PDE in equation 15 along with initial conditions (equation 18) and thermal insulated boundary conditions (equation 19) can be solved using the method of separation of variables. The solution involves 3 steps. (i) convert the PDE into two separate ODEs, (ii) solve the two ODEs and (iii) compose the solutions to the two ODEs into a solution of the original PDE. Temperature as function of two variables can be written as product of two separate functions, each of one variable.

$$T(x,t) = F(x)\,.\,G(t) \ldots\ldots\ldots (20)$$

The equation 15 then can be written as follows by putting lattice temperature as product of two separate functions F and G. For simplicity the value of S is assumed to be zero.

$$CF\frac{dG}{dt} + vF\frac{d^2G}{dt^2} = kG\frac{d^2F}{dx^2} + \mu k\frac{\partial^2}{\partial x^2}\left(F\frac{dG}{dt}\right)$$

$$CF\frac{dG}{dt} + vF\frac{d^2G}{dt^2} = kG\frac{d^2F}{dx^2} + \mu k\frac{dG}{dt}\frac{d^2F}{dx^2}$$

$$F(C\frac{dG}{dt} + v\frac{d^2G}{dt^2}) = \frac{d^2F}{dx^2}(kG + \mu k\frac{dG}{dt})$$

$$\frac{1}{F}\frac{d^2F}{dx^2} = \frac{1}{\left(kG + \mu k\frac{dG}{dt}\right)}\left(C\frac{dG}{dt} + v\frac{d^2G}{dt^2}\right) = constant$$

The constant can be positive, zero or negative but from the previous calculations we saw that taking constant value positive or zero violate the boundary condition or cannot validate the equation for all time instants. Therefore, let the constant be $-\lambda$. Then solving for two part we get two equations of which one is time dependent and the other is time independent.

$$\frac{1}{F}\frac{d^2F}{dx^2} = -\lambda$$

$$\frac{d^2F}{dx^2} + \lambda F = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(21a)$$

$$\frac{1}{\left(kG + \mu k\frac{dG}{dt}\right)}\left(C\frac{dG}{dt} + v\frac{d^2G}{dt^2}\right) = -\lambda$$

$$v\frac{d^2G}{dt^2} + (C + \lambda\mu k)\frac{dG}{dt} + \lambda kG = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (21b)$$

The solution of equation 21a is given by:

$$F = Acos\left(\lambda^{\frac{1}{2}}x\right) + Bsin\left(\lambda^{\frac{1}{2}}x\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(22)$$

Differentiating equation 22 with respect to x we get

$$\frac{dF}{dx} = -\lambda^{\frac{1}{2}}A\ sin\left(\lambda^{\frac{1}{2}}x\right) + \lambda^{\frac{1}{2}}B\ cos\left(\lambda^{\frac{1}{2}}x\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(23)$$

Applying boundary condition at the front surface (x=0)

$$\frac{dF}{dx}(x = 0) = 0 = -\lambda^{\frac{1}{2}}A\ sin(0) + \lambda^{\frac{1}{2}}B\ cos(0)$$

$$\lambda^{\frac{1}{2}}B = 0$$

But λ is constant and must not be zero. Therefore $B = 0$.

Then we have

$$F = Acos\left(\lambda^{\frac{1}{2}}x\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(24)$$

Applying boundary condition at the back surface (x=L)

$$\frac{dF}{dx}(x = L) = 0 = -\lambda^{\frac{1}{2}}A\ sin\left(\lambda^{\frac{1}{2}}L\right)$$

$$sin\left(\lambda^{\frac{1}{2}}L\right) = \sin\,(j\pi)$$

$$\lambda_j = (\frac{j\pi}{L})^2$$

Where j = 0, 1, 2, ………………

The equation 24 then can be written as:

$$F(x) = Acos\left(\frac{j\pi}{L}x\right)$$

$$F(x) = A_0cos(0) + A_1\cos\left(\frac{\pi}{L}x\right) + A_2\cos\left(\frac{2\pi}{L}x\right) + \cdots \ldots\ldots\ldots\ldots\ldots$$

$$F(x) = A_0 + \sum_{j=1}^{\infty} A_j\,cos\left(\frac{j\pi}{L}x\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (25)$$

The solution of equation 21b is given by,

$$G(t) = B_1e^{m_1t} + B_2e^{m_2t} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (26)$$

Where, $m_1 = \frac{-(C+\lambda_j\mu k)+\sqrt{(C+\lambda_j\mu k)^2-4\lambda_j vk}}{2v}$ and $m_2 = \frac{-(C+\lambda_j\mu k)-\sqrt{(C+\lambda_j\mu k)^2-4\lambda_j vk}}{2v}$

Applying the first initial condition we have

$$G(t=0) = 0 = B_1 + B_2$$

Or, $B_2 = -B_1$

Then the equation 26 becomes:

$$G(t) = B_1(e^{m_1t} - e^{m_2t}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (27)$$

For $j = 0;\;\; m_1 = 0\; and\; m_2 = -\frac{C}{v}$

Equation 27 then can be rewritten as:

$$G(t) = B_0\left(1 - e^{-\frac{Ct}{v}}\right) + \sum_{j=1}^{\infty} B_j\,(e^{m_1t} - e^{m_2t}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (28)$$

The general solution for the lattice temperature is then obtained by multiplying equations 25 and 28.

$$T_l(x,t) = D_0\left(1 - e^{-\frac{Ct}{v}}\right) + \sum_{j=1}^{\infty} D_j\,(e^{m_1t} - e^{m_2t})cos\left(\frac{j\pi}{L}x\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (29)$$

The electron temperature distribution can be obtained from equation 11

$$T_e(x,t) = \frac{C_l}{g}\frac{\partial T_l(x,t)}{\partial t} + T_l(x,t) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (30)$$

Differentiating equation 29 with respect to time we have

$$\frac{\partial T_l(x,t)}{\partial t} = \frac{D_0 C}{v} e^{-\frac{Ct}{v}} + \sum_{j=1}^{\infty} D_j\,(m_1 e^{m_1 t} - m_2 e^{m_2 t}) cos\left(\frac{j\pi}{L}x\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(31)$$

Combining equation 29, 30 and 31 we get the equation for electron temperature

$$T_e(x,t) = \frac{\mu D_0 C}{v} e^{-\frac{Ct}{v}} + \mu \sum_{j=1}^{\infty} D_j\,(m_1 e^{m_1 t} - m_2 e^{m_2 t}) cos\left(\frac{j\pi}{L}x\right) + T_l(x,t) \ldots\ldots\ldots\ldots\ldots\ldots.(32)$$

Using equation 18b (second initial condition) and equation 31 we have

$$\frac{\partial T_l(x,0)}{\partial t} = \frac{D_0 C}{v} + \sum_{j=1}^{\infty} D_j\,(m_1 - m_2) cos\left(\frac{j\pi}{L}x\right) = \frac{(1-R)J}{vd} \exp\left(-\frac{x}{d}\right)$$

Taking integration on both sides from 0 to L we have

$$\int_0^L \frac{D_0 C}{v} dx + \int_0^L \sum_{j=1}^{\infty} D_j\,(m_1 - m_2) cos\left(\frac{j\pi}{L}x\right) dx = \int_0^L \frac{(1-R)J}{vd} \exp\left(-\frac{x}{d}\right) dx \ldots\ldots.(33)$$

$$\frac{D_0 C}{v}[L-0] + \sum_{j=1}^{\infty} D_j\,(m_1 - m_2)\frac{L}{j\pi}[\sin(j\pi) - \sin(0)] = \frac{(1-R)J}{vd}(-d)[\exp\left(-\frac{L}{d}\right) - \exp\,(0)]$$

Since j is an integer $\sin(j\pi) = 0$, then we have

$\frac{D_0 CL}{v} + 0 = \frac{(1-R)J}{v}[1 - \exp\,(-\frac{L}{d})]$

Or,

$$D_0 = \frac{(1-R)J}{LC}\left(1 - e^{-\frac{L}{d}}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(34)$$

Now to determine the coefficient D_j multiply both sides of equation 33 by $cos\left(\frac{l\pi}{L}x\right)$ we can write

$$\int_0^L \frac{D_0 C}{v} cos\left(\frac{l\pi}{L}x\right) dx + \int_0^L \sum_{j=1}^{\infty} D_j\,(m_1 - m_2) cos\left(\frac{j\pi}{L}x\right) cos\left(\frac{l\pi}{L}x\right) dx = \int_0^L \frac{(1-R)J}{vd} \exp\left(-\frac{x}{d}\right) cos\left(\frac{l\pi}{L}x\right) dx$$

This equation has three integrals are evaluated separately. Let's the integrals are $I_1, I_2, and\ I_3$

$$I_1 + I_2 = I_3 \ldots\ldots\ldots\ldots\ldots\ldots\ldots(35)$$

Where, $I_1 = \int_0^L \frac{D_0 C}{v} cos\left(\frac{l\pi}{L}x\right) dx \ldots \ldots \ldots \ldots \ldots \ldots .. (36a)$

$$I_2 = \int_0^L \sum_{j=1}^{\infty} D_j\ (m_1 - m_2) cos\left(\frac{j\pi}{L}x\right) cos\left(\frac{l\pi}{L}x\right) dx\ \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (36b)$$

$$I_3 = \int_0^L \frac{(1-R)J}{vd} \exp\left(-\frac{x}{d}\right) cos\left(\frac{l\pi}{L}x\right) dx \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (36c)$$

From equation 36a

$$I_1 = \frac{D_0 C}{v} [\sin(l\pi) - \sin(0)] \frac{L}{l\pi}$$

Since l is an integer $\sin(l\pi) = 0$, then we have

$$I_1 = 0$$

In equation 36b, the integrand is a product of two even functions which are mutually orthogonal. To determine the integral, we need to consider two cases (since the integer j ranges from zero to infinitive): $j = l\ and\ j \neq l$.

For $j = l$

$$I_2 = \int_0^L \sum_{j=1}^{\infty} D_j\ (m_1 - m_2) cos^2\left(\frac{j\pi}{L}x\right) dx$$

$$I_2 = \frac{1}{2}\sum_{j=1}^{\infty} D_j\ (m_1 - m_2) \int_0^L \left(1 + cos\left(\frac{2j\pi}{L}x\right)\right) dx$$

$$I_2 = \frac{1}{2}\sum_{j=1}^{\infty} D_j\ (m_1 - m_2) \left[\left(L + \frac{L}{2j\pi}\sin(2j\pi)\right) - \left(0 + \frac{L}{2j\pi}\sin(0)\right)\right]$$

Since j is an integer $\sin(2j\pi) = 0$, then we have

$$I_2 = \frac{1}{2}\sum_{j=1}^{\infty} D_j\ (m_1 - m_2) L \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . (37a)$$

Now for $j \neq l$

$$I_2 = \int_0^L \sum_{j=1}^{\infty} D_j\ (m_1 - m_2) cos\left(\frac{j\pi}{L}x\right) cos\left(\frac{l\pi}{L}x\right) dx$$

$$I_2 = \sum_{j=1}^{\infty} D_j\ (m_1 - m_2) \frac{1}{2} \int_0^L 2cos\left(\frac{j\pi}{L}x\right) cos\left(\frac{l\pi}{L}x\right) dx$$

$$I_2 = \sum_{j=1}^{\infty} D_j\ (m_1 - m_2)\frac{1}{2}\int_0^L cos\left(\frac{(j-l)\pi}{L}x\right) + cos\left(\frac{(j+l)\pi}{L}x\right)dx$$

$$I_2 = \sum_{j=1}^{\infty} D_j\ (m_1 - m_2)\frac{1}{2}\ [\left(\frac{L}{(j-l)\pi}\sin(j-l)\,\pi + \frac{L}{(j+l)\pi}\sin(j+l)\,\pi\right) - (\frac{L}{(j-l)\pi}\sin(0) + \frac{L}{(j+l)\pi}\sin\,(0))]$$

Since j and l both are integers and so (j-l) and (j+l) are also integers then $\sin(j-l)\,\pi = \sin(j+l)\,\pi = 0$, and we have

$$I_2 = 0 \ldots\ldots..(37b)$$

A function of two variables is called Kronecker Delta function if its value is 1 when the variables are equal and 0 otherwise. The integral I_2 then can be expressed as

$$I_2 = \frac{1}{2}\sum_{j=1}^{\infty} D_j\ (m_1 - m_2)\frac{L}{2}\delta_{j,l}$$

Where, $\delta_{j,l}$ is the Kronecker Delta function. Then we have

$$I_2 = D_j(m_1 - m_2)\frac{L}{2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(38)$$

From equation 36c

$$I_3 = \int_0^L \frac{(1-R)J}{vd}\exp\left(-\frac{x}{d}\right)cos\left(\frac{l\pi}{L}x\right)dx$$

$$I_3 = \int_0^L \frac{(1-R)J}{vd}\exp\left(-\frac{x}{d}\right)\frac{1}{2}[\exp\left(\frac{il\pi}{L}\right)x + \exp\left(\frac{-il\pi}{L}\right)x]dx$$

$$I_3 = \frac{(1-R)J}{2vd}\int_0^L [\exp\left(-\frac{1}{d}+\frac{il\pi}{L}\right)x + \exp\left(-\frac{1}{d}-\frac{il\pi}{L}\right)x]dx$$

$$I_3 = \frac{(1-R)J}{2vd}[\frac{\exp\left(-\frac{L}{d}+\frac{il\pi}{L}\right)L}{\left(-\frac{1}{d}+\frac{il\pi}{L}\right)} + \frac{\exp\left(-\frac{L}{d}-\frac{il\pi}{L}\right)L}{\left(-\frac{1}{d}-\frac{il\pi}{L}\right)} - \frac{1}{\left(-\frac{1}{d}+\frac{il\pi}{L}\right)} - \frac{1}{\left(-\frac{1}{d}-\frac{il\pi}{L}\right)}]$$

$$I_3 = \frac{(1-R)J}{2vd}[\frac{\exp\,(-\frac{L}{d})\ \exp\,(il\pi)}{-\frac{1}{d}\left(1-\frac{il\pi d}{L}\right)} + \frac{\exp\,(-\frac{L}{d})\ \exp\,(-il\pi)}{-\frac{1}{d}\left(1+\frac{il\pi d}{L}\right)} - \frac{1}{-\frac{1}{d}\left(1-\frac{il\pi d}{L}\right)} - \frac{1}{-\frac{1}{d}\left(1+\frac{il\pi d}{L}\right)}]$$

$$I_3 = \frac{-(1-R)J}{2v}[\frac{\exp\left(-\frac{L}{d}\right)((\exp(il\pi)\left(1+\frac{il\pi d}{L}\right) + \exp(-il\pi)\left(1-\frac{il\pi d}{L}\right))}{\left(1-\frac{il\pi d}{L}\right)\left(1+\frac{il\pi d}{L}\right)} - \frac{\left(1+\frac{il\pi d}{L}\right)+\left(1-\frac{il\pi d}{L}\right)}{\left(1-\frac{il\pi d}{L}\right)\left(1+\frac{il\pi d}{L}\right)}]$$

$$I_3 = \frac{-(1-R)J}{2v}[\frac{\exp\left(-\frac{L}{d}\right)[(\exp(il\pi)+\exp(-il\pi)) + \frac{il\pi d}{L}(exp(il\pi) - \exp(-il\pi))]}{1+(\frac{l\pi d}{L})^2} - \frac{2}{1+(\frac{l\pi d}{L})^2}]$$

$$I_3 = \frac{-(1-R)J}{2v}[\frac{\exp\left(-\frac{L}{d}\right)(2\cos(l\pi) + \frac{il\pi d}{L}2\sin(l\pi))}{1+(\frac{l\pi d}{L})^2} - \frac{2}{1+(\frac{l\pi d}{L})^2}]$$

Since l is an integer, $\sin(l\pi) = 0$, we have

$$I_3 = \frac{-(1-R)J}{2v}[\frac{\exp\left(-\frac{L}{d}\right)2\cos(l\pi)}{1+(\frac{l\pi d}{L})^2} - \frac{2}{1+(\frac{l\pi d}{L})^2}]$$

$$I_3 = \frac{-(1-R)J}{2v}[\frac{\exp\left(-\frac{L}{d}\right)2\cos(l\pi) - 2}{1+(\frac{l\pi d}{L})^2}$$

$$I_3 = \frac{(1-R)J}{v}[\frac{1-\exp\left(-\frac{L}{d}\right)\cos(l\pi)}{1+\left(\frac{l\pi d}{L}\right)^2}]$$

Since l is just an index it can be defined to be anything, $l = j$, then we can write the above equation as:

$$I_3 = \frac{(1-R)J}{v}\left[\frac{1-\exp\left(-\frac{L}{d}\right)\cos(j\pi)}{1+\left(\frac{j\pi d}{L}\right)^2}\right] \dots\dots\dots\dots\dots\dots\dots\dots\dots..(39)$$

Now substituting for $I_1, I_2, and\ I_3$ into equation 35 we have

$$0 + D_j(m_1 - m_2)\frac{L}{2} = \frac{(1-R)J}{v}\left[\frac{1-\exp\left(-\frac{L}{d}\right)\cos(j\pi)}{1+\left(\frac{j\pi d}{L}\right)^2}\right]$$

And finally,

$$D_j = \frac{2(1-R)J}{(m_1-m_2)Lv}\left[\frac{1-\exp\left(-\frac{L}{d}\right)\cos(j\pi)}{1+\left(\frac{j\pi d}{L}\right)^2}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (40)$$

Finally, the solution obtained as:

$$T_l(x,t) = D_0\left(1-e^{-\frac{Ct}{v}}\right) + \sum_{j=1}^{\infty} D_j\,(e^{m_1 t} - e^{m_2 t})cos\left(\frac{j\pi}{L}x\right)$$

$$T_e(x,t) = \frac{\mu D_0 C}{v}e^{-\frac{Ct}{v}} + \mu\sum_{j=1}^{\infty} D_j\,(m_1 e^{m_1 t} - m_2 e^{m_2 t})cos\left(\frac{j\pi}{L}x\right) + T_l(x,t)$$

$$D_0 = \frac{(1-R)J}{LC}\left(1-e^{-\frac{L}{d}}\right)$$

$$D_j = \frac{2(1-R)J}{(m_1-m_2)Lv}\left[\frac{1-\exp\left(-\frac{L}{d}\right)\cos(j\pi)}{1+\left(\frac{j\pi d}{L}\right)^2}\right]$$

$$\lambda_j = (\frac{j\pi}{L})^2$$

$$m_1 = \frac{-(C+\lambda_j\mu k) + \sqrt{(C+\lambda_j\mu k)^2 - 4\lambda_j v k}}{2v}$$

$$m_2 = \frac{-(C+\lambda_j\mu k) - \sqrt{(C+\lambda_j\mu k)^2 - 4\lambda_j v k}}{2v}$$

MATLAB Code:

```
clc

clear


% Putting Constant Values

L= 1e-6;          % Thickness of metal sample is 1 um

tend= 1e-9;        % Diffusion upto 1 ns

R= 0.9;
```

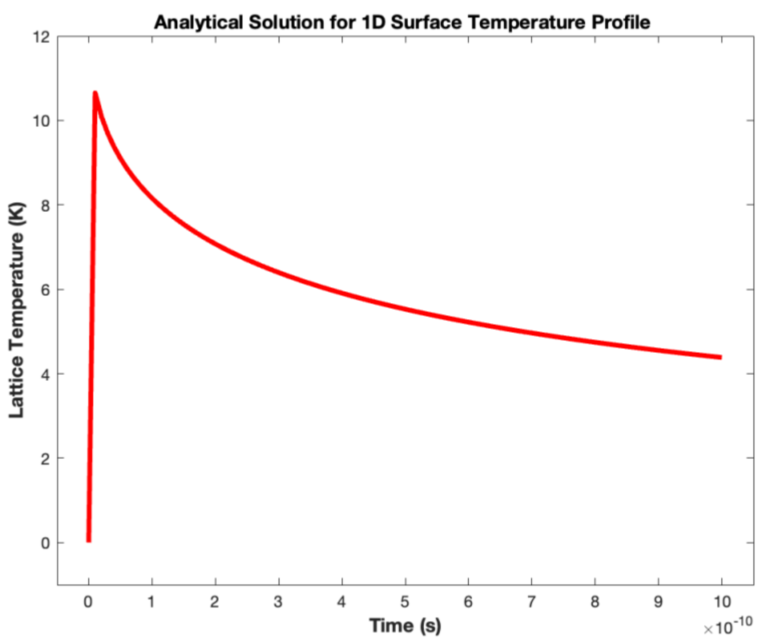
```
J=4.8;
d= 15e-9;
g= 17e17;
k=55;
Ce= 3.0e5;
Cl= 2.3e6;
N=500;

% Calculation of other constant
C= Ce+Cl;
Mu= Cl/g;
Nu= (Ce*Cl)/g;
Dnot= (((1-R)*J)/(L*C))*(1-exp(-L/d));



%Mesh spacing and time steps
nx=100;
nt=100;
dx= L/(nx-1);
dt=tend/(nt-1);

% Creating arrays to save data
y= linspace (0, L, nx);
t= linspace (0, tend, nt);



% Memory preallocation
Tl=zeros(nx, nt);
Te=zeros(nx, nt);

for i=1:nt
   ti=(dt*i)-dt;
```

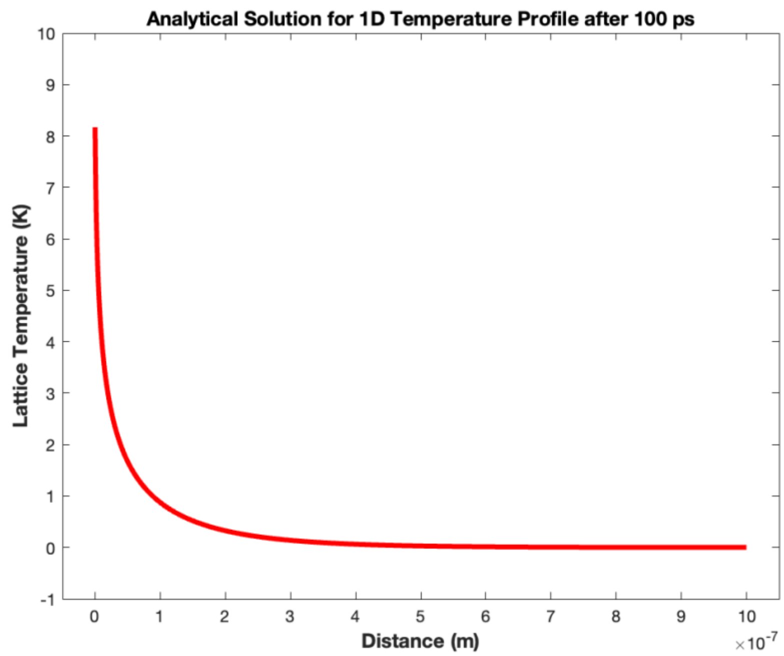
```
    for r=1:nx
        xr=(dx*r)-dx;

        newsumTl=0.0;
        newsumTe=0.0;
        for j=1:N
            Lamda=((j*pi)/L)^2;
            P=C+(Lamda*Mu*k);
            Q=4*Lamda*Nu*k;
            m1=(-P+sqrt(P^2-Q))/(2*Nu);
            m2=(-P-sqrt(P^2-Q))/(2*Nu);
            A=1-((exp(-L/d))*cos(j*pi));
            B=1+((d*j*pi)/L)^2;
            D=(2*(1-R)*J*A)/((m1-m2)*L*Nu*B);
            sumtermTl=D*(exp(m1*ti)-exp(m2*ti))*cos((j*pi*xr)/L);
            sumtermTe=D*(m1*exp(m1*ti)-m2*exp(m2*ti))*cos((j*pi*xr)/L);
            newsumTl=newsumTl+sumtermTl;
            newsumTe=newsumTe+sumtermTe;
        end
        Tl(r, i)=Dnot*(1-exp((-C*ti)/Nu))+newsumTl;
        Te(r, i)=(Mu*Dnot*C*exp(-(C*ti)/Nu))/Nu + Mu*newsumTe + Dnot*(1-exp((-C*ti)/Nu))+newsumTl;

    end



end
```

```
% Plotting temperature profile as a function of time
    plot(t,Tl(1, :),'r','linewidth', 3)
    axis([-50e-12 1050e-12 -1 12]);
    title('Analytical Solution for 1D Surface Temperature Profile ','fontweight', 'bold','FontSize',12)
    xlabel('Time (s)','fontweight','bold','FontSize',12)
    ylabel('Lattice Temperature (K)','fontweight', 'bold','FontSize',12)


% Plotting temperature profile as a function of Distance
    plot(y,Tl(:, 100),'r','linewidth', 3)
    axis([-50e-9 1050e-9 -1 10]);
    title('Analytical Solution for 1D Temperature Profile after 100 ps','fontweight', 'bold','FontSize',12)
    xlabel('Distance (m)','fontweight','bold','FontSize',12)
    ylabel('Lattice Temperature (K)','fontweight', 'bold','FontSize',12)


% A surface plot is often a good way to study a solution.
    surf(y, t, Tl)
    title('Analytical Solution of 1D Heat equation','fontweight', 'bold','FontSize',12)
    xlabel('Distance x (m)','fontweight', 'bold','FontSize',12)
    ylabel('Time t (s)','fontweight', 'bold','FontSize',12)
    zlabel('Lattice Temperature T (K)','fontweight', 'bold','FontSize',12)

% Plotting temperature profile as a function of time
    plot(t,Te(1, :),'r','linewidth', 3)
    axis([-50e-12 1050e-12 -10 120]);
    title('Analytical Solution for 1D Surface Temperature Profile ','fontweight', 'bold','FontSize',12)
    xlabel('Time (s)','fontweight','bold','FontSize',12)
    ylabel('Electron Temperature (K)','fontweight', 'bold','FontSize',12)


% Plotting temperature profile as a function of Distance
    plot(y,Tl(:, 100),'r','linewidth', 3)
```

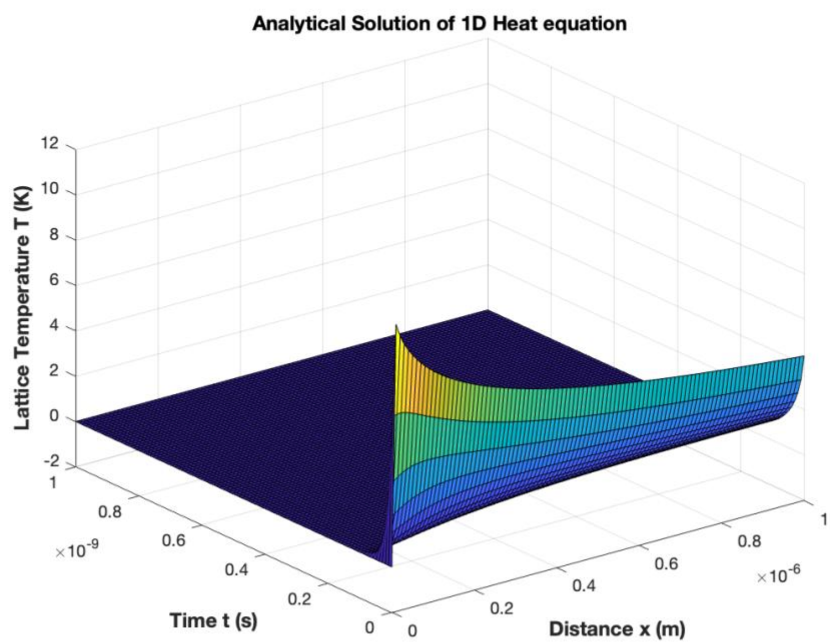
```
axis([-50e-9 1050e-9 -1 10]);
title('Analytical Solution for 1D Temperature Profile after 100 ps','fontweight', 'bold','FontSize',12)
xlabel('Distance (m)','fontweight','bold','FontSize',12)
ylabel('Electron Temperature (K)','fontweight', 'bold','FontSize',12)


% A surface plot is often a good way to study a solution.
surf(y, t, Te)
title('Analytical Solution of 1D Heat equation','fontweight', 'bold','FontSize',12)
xlabel('Distance x (m)','fontweight', 'bold','FontSize',12)
ylabel('Time t (s)','fontweight', 'bold','FontSize',12)
zlabel('Electron Temperature T (K)','fontweight', 'bold','FontSize',12)
```

Results:

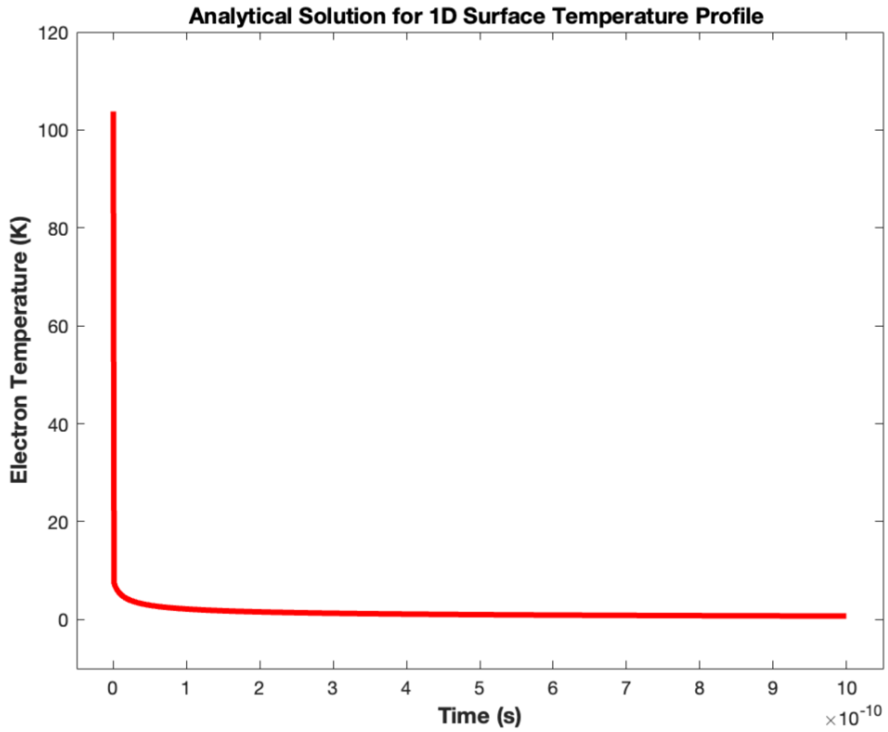


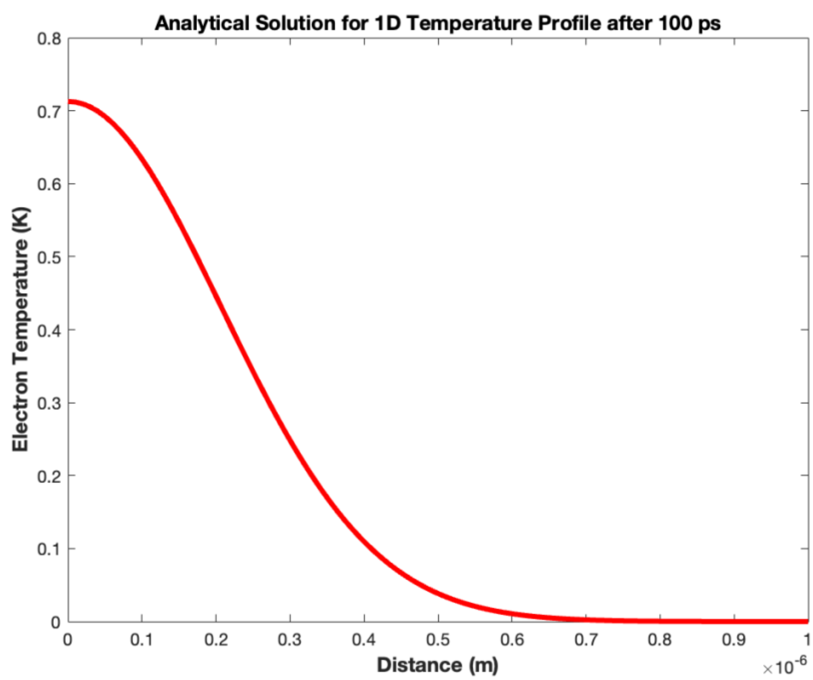


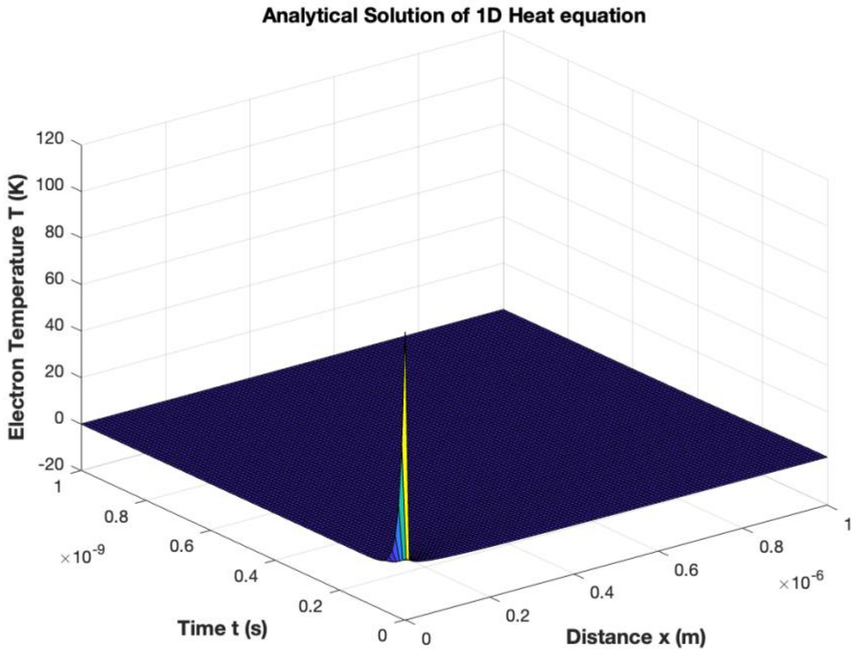
Analytical Solution for 1D Temperature Profile after 100 ps
Lattice Temperature (K)
10
9
8
7
6
5
4
3
2
1
0
-1
0
1
2
3
4
5
6
7
8
9
10
Distance (m)
×10^-7



Analytical Solution of 1D Heat equation
Lattice Temperature T (K)
12
10
8
6
4
2
0
-2
Time t (s)
×10^-9
1
0.8
0.6
0.4
0.2
0
Distance x (m)
×10^-6
0
0.2
0.4
0.6
0.8
1


Analytical Solution for 1D Surface Temperature Profile
Electron Temperature (K)
Time (s)
×10^-10
0
1
2
3
4
5
6
7
8
9
10
120
100
80
60
40
20
0


Analytical Solution for 1D Temperature Profile after 100 ps
Electron Temperature (K)
Distance (m)
×10^-6
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



Analytical Solution of 1D Heat equation
Electron Temperature T (K)
120
100
80
60
40
20
0
-20
1
0.8
0.6
0.4
0.2
0
×10-9
Time t (s)
0
0.2
0.4
0.6
0.8
1
×10-6
Distance x (m)