MME 9621
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Department of Mechanical and Material Engineering

Computational Methods: Course Project

MME-9621

Course Instructor- Prof. Hossain

Project Topic: "Numerical Modelling of Temperature around a nuclear waste rod"

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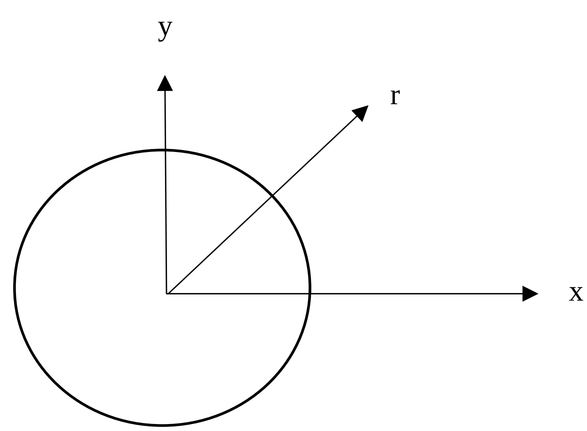
1. Problem Statement:

The temperature around nuclear waste rods are not only interesting physics problem but also important for safety concern that must be addressed before building a nuclear waste storage. Problem involved for the Project is based on Transient 2D heat conduction problem of Temperature distribution around a nuclear waste rod. The task of the project is to develop a MATLAB code based on finite difference method for the variation of Temperature distribution around the nuclear waste with respect to time interval. The mathematical model involves the Transient 2D Poisson equation which is given below:

$$\underbrace{\frac{1}{k}\frac{\partial T}{\partial t}(r,t) - \nabla^2 T(r,t)}_{\textit{2-D heat equation}} = \underbrace{S(r,t)}_{\textit{Source Term}}$$



Where, r=a

Figure 1. Nuclear rod buried in ground

Where source Term due to the radioactive decay of rod is given by:

$$S(r,t) = \begin{cases} T_{rod}{}^{e^{-t/\tau_o}} \big/ a^2 & for\ r \leq a \\ 0 & elsewhere \end{cases}$$

Where a= 25 cm, k =2 x 10^7 cm^2/year, T_{rod} = 1K, $\tau_o = 100\ years$, r_c=100cm, T_E = 300K, 0<r<100cm and 0<t<100 years. Initially T (r, t=0) =300K

Furthermore, the temperature distribution obtained from the MATLAB solver will be compared with other numerical methods such as implicit, explicit and for the time discretization accuracy, crank Nicolson method can be used.

2. Detailed Mathematical procedure and Numerical algorithm

2.1 Mathematical Procedure and Boundary Conditions

The problem has circular symmetry (i.e. no $\emptyset\ dependence$) 2-D problem in (x, y) reduced to 1-D problem in r. $\nabla^2 T = T_{xx} + T_{yy}$ is 2-D in cartesian co-ordinates. However, if we choose to use polar co-ordinates then the temperature, T (r, t) is a function of r and t only because the rod circular symmetric and there is no $\emptyset\ dependence$. This reduces the original 2-D problem to 1-D.

$$\begin{aligned} T_{xx} &= \frac{\partial^2 T}{\partial x^2} = (\cos\phi\frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial\phi})(\cos\phi\frac{\partial T}{\partial r} - \frac{\sin\phi}{r}\frac{\partial T}{\partial\phi}) \\ &= \cos^2\phi T_{rr} - \frac{2\sin\phi\cos\phi}{r}T_{r\phi} + \frac{\sin^2\phi}{r}T_r + \frac{2\cos\phi\sin\phi}{r}T_\phi + \frac{\sin^2\phi}{r}T_{\phi\phi} \end{aligned}$$

$$\begin{aligned} T_{yy} &= (\sin\phi\frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial\phi})(\sin\phi\frac{\partial T}{\partial r} + \frac{\cos\phi}{r}\frac{\partial T}{\partial\phi}) \\ &= \sin^2\phi T_{rr} + \frac{2\cos\phi\sin\theta}{r}T_{r\phi} - \frac{2\cos\phi\sin\phi}{r^2}T_\phi + \frac{\cos^2\phi}{r}T_r + \frac{\cos^2\phi}{r^2}T_{\phi\phi} \end{aligned}$$

$$\text{and } T_{xx} + T_{yy} = T_{rr} + \frac{1}{r}T_r + \frac{1}{r}^2 T_{\phi\phi}$$

Using $cos^2\emptyset + sin^2\emptyset = 1$

Since the temperature has no $\emptyset\ dependence$. Then in that case $T_{\emptyset\emptyset} = 0$. Therefore, we will solve the 1-D heat equation in polar co-ordinates.

$$\frac{1}{k}\frac{\partial T}{\partial t}(r,t) - \frac{\partial^2 T}{\partial^2 r} - \frac{1}{r}\frac{\partial T}{\partial r} = S(r,t)$$

From the above equation, it can be noticed that if r=0 then there is a singularity. This point must be taken into consideration for the convergence of the solution.

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We know that the nuclear rod is no longer radioactive and stops releasing heat if $S(r,t) = 0$ as t=∞ and far away from the rod the temperature equals to the ambient condition therefore, T (r =r_c, t) = 300K. therefore, the solution should approach the ambient temperature equals the ambient temperature T (r, t) = 300K when rod has finished radioactive decaying.

We will solve this partial differential equation with the help of finite difference schemes.

Initial condition T(r,0) = 300K

Neuman boundary conditions at r = 0.

$$\frac{\partial T}{\partial r}(r = 0, t) = 0$$

Dirichlet boundary conditions at r = r_c

T (r=r_c, t) = 300K

$$\Delta r = \frac{r_c}{x+1}, \Delta t = \frac{t_f}{m}, r_i = i\Delta r, 0 \le i \le x+1, t_n = k\Delta t, 0 \le k \le m, T(r_i, t_n) = T_i{}^n \; and \; S(r_i, t_n) = S^n{}_i$$

For boundary condition evaluation, we can solve Dirichlet boundary condition using finite difference scheme for discrete Neuman boundary condition as given below:

At r=0

$$\frac{\partial T}{\partial r}(r = 0, t) = \frac{T^n{}_1 - T^n{}_0}{\Delta r} = 0$$

$$\boldsymbol{T^n{}_1 = T^n{}_0}$$

Discrete Dirichlet Boundary condition at r = r_c become

$$T^n{}_i\,(r = r_c, t) = \; T^n{}_{x+1} = 300$$

2.2 Numerical Solution and Discretization

Finite difference schemes for **Backward Euler Implicit Method**

Discretization of the partial differential equation into algebraic equation;

$$\frac{1}{k}\frac{\partial T}{\partial t}(r,t) - \frac{\partial^2 T}{\partial^2 r} - \frac{1}{r}\frac{\partial T}{\partial r} = S(r,t)$$

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$\frac{\partial T}{\partial t} = \frac{T_i{}^{n+1} - T_i{}^n}{\Delta t}$

$\frac{\partial^2 T}{\partial r^2} = \frac{T_{i-1}{}^{n+1} - 2T_i{}^{n+1} + T_{i+1}{}^{n+1}}{(\Delta r)^2}$ [Center Difference in Space]

$\frac{\partial T}{\partial r} = \frac{T^{n+1}{}_{i+1} - T^{n+1}{}_{i-1}}{2\Delta r}$ [Leap frog method in space]

$\frac{1}{k}\frac{T_i{}^{n+1} - T_i{}^n}{\Delta t} - \frac{T_{i-1}{}^{n+1} - 2T_i{}^{n+1} + T_{i+1}{}^{n+1}}{(\Delta r)^2} - \frac{1}{r}\frac{T^{n+1}{}_{i+1} - T^{n+1}{}_{i-1}}{2\Delta r} = S_i{}^n$

By rearranging we get,

$\frac{1}{K\Delta t}\left(T_i{}^{n+1} - T_i{}^n\right) - \frac{1}{(\Delta r)^2}\left(T_{i-1}{}^{n+1} - 2T_i{}^{n+1} + T_{i+1}{}^{n+1}\right) - \frac{1}{r2\Delta r}\left(T^{n+1}{}_{i+1} - T^{n+1}{}_{i-1}\right) = S_i{}^n$

Let us consider, $\beta = \frac{k\Delta t}{\Delta r^2}$

$T^{n+1}{}_{i+1}\left(-\beta - \frac{\beta}{2i}\right) + T^{n+1}{}_{i-1}\left(-\beta + \frac{\beta}{2i}\right) + T^{n+1}{}_i(1 + 2\beta) = T^n{}_i + S_i{}^n k\Delta t$

For I = 5 interior points

Matrix A=

$$\begin{matrix} 1+2*\mathrm{Beta} & -beta-beta/2i & 0 & 0 & 0 \\ -beta+beta/2i & 1+2beta & -beta-beta/2i & 0 & 0 \\ 0 & -beta+beta/2i & 1+2beta & -beta-beta/2i & 0 \\ 0 & 0 & -beta+beta/2i & 1+2beta & -beta-beta/2i \\ 0 & 0 & 0 & -beta+beta/2i & 1+2beta \end{matrix}$$

Matrix “x” Column Vector

= [T_1^{n+1} ; T_2^{n+1} ; T_2^{n+1} ; T_3^{n+1} ; T_4^{n+1} ; T_5^{n+1}] + [(-beta+ beta/2i) T_0^{n+1} ;0 ; 0 ; 0 ; 0 ; (-beta- beta/2i) T_6^{n+1}]

Matrix « b »

$[T_1^n ; T_2^n ; T_2^n ; T_3^n ; T_4^n ; T_5^n] + k\Delta t[S_1{}^n; S_2{}^n; S_3{}^n; S_4{}^n; S_5{}^n]$

2.3 Method Selection

The above discretization for space into 5 nodes and the matrix obtained is banded matrix and bandwidth of 3. This means it is a tridiagonal matrix and to reduce computational time it is better to use tridiagonal solver directly instead using MATLAB backslash operator. On the other hand, we will apply backward Euler implicit method to solve the temperature distribution over the nuclear waste rod. We know that the implicit is conditionally stable and there is no discretization restriction on space and time. However, the computational time is more than explicit method but we know that solution must be converged in implicit method. The accuracy in time O (Δt) and for space accuracy is second order O$(\Delta x)^2$

2.4 Numerical Algorithm

In numerical analysis, our first step is to obtained grid independence test and we know that temperature is 2 digit accurate therefore grid independence test can be obtained with two-digit accuracy.

These are the results for 5 nodes in the space these graphs will be compared with results obtained at higher number of nodes.

```
r1=0;
rc=100.;
r2=rc;

T = 100.;

n = 99;
m = 1000.;

dr = rc/(n+1.);
dt = T/m;



t=0.;

kappa = 2.e7;

s = kappa*dt/(dr^2);
```

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```
A=zeros(n,n);

for i = 1:n
    for j = 1:n

        if i==j
           A(i,j) = 1. + 2.*s;
        elseif i==j-1
           A(i,j) = -s - s/(2.*i);
        elseif i==j+1
           A(i,j) = -s + s/(2.*i);
        else
           A(i,j) = 0.;
        end
    end
end


A(1,1) = 1+s+s/2;

b= zeros(n,1);


b(n) = -(-s-s/(2*n))*300.;


r = linspace(r1+dr,r2-dr, n)';



T_tk = 300.*ones(n,1);

figure(1)
plot (r,T_tk,'-')
title ('Initial condition for Temperature distribution')
xlabel ('r')
ylabel ('Temperature')


Temp=zeros(n,m);
tvec=zeros(m,1);

Temp(:,1) = T_tk;
tvec(1) = t;


source_vector = zeros(n,1);
a_source = 25.;
Trod = 1.;
```

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```
tau_0 = 100;
for i = 1:n
    if r(i) < a_source
       source_vector(i) = 1;
    end
end

temp_solutions=zeros(4,1);
isolution = 1;

for k = 1:m
    t = t+dt;
    source = (Trod*exp(-t/tau_0)/(a_source^2))*source_vector;

    c = T_tk + b + kappa*dt*source;
    T_tk_1 = A\c;


    Temp(:,k) = T_tk_1;


    T_tk = T_tk_1;
    tvec(k) = t;



    if k==10
       temp_solutions(isolution) = t
       isolution = isolution+1;
       Temp1year = T_tk_1;
    elseif k==100
       temp_solutions(isolution) = t
       isolution = isolution+1;
       Temp10year = T_tk_1;
    elseif k==500
       temp_solutions(isolution) = t
       isolution = isolution+1;
       Temp50year = T_tk_1;
    elseif k==1000
       temp_solutions(isolution) = t
       isolution = isolution+1;
       Temp100year = T_tk_1;
    end

end



figure(2)
mesh (tvec,r,Temp)
title ('Variation of Temperature distribution with time using Backward Euler
method')
```

```
xlabel ('t')
ylabel ('r')
zlabel ('Temperature')


figure(3)

plot(r,Temp1year,r,Temp10year,r,Temp50year,r,Temp100year)

legend ('Temp after 1 year', 'Temp after 10 years', 'Temp after 50 years',
'Temp after 100 years')

xlabel ('r')
ylabel ('Temperature')
```

2.4.1 Grid Independence Test

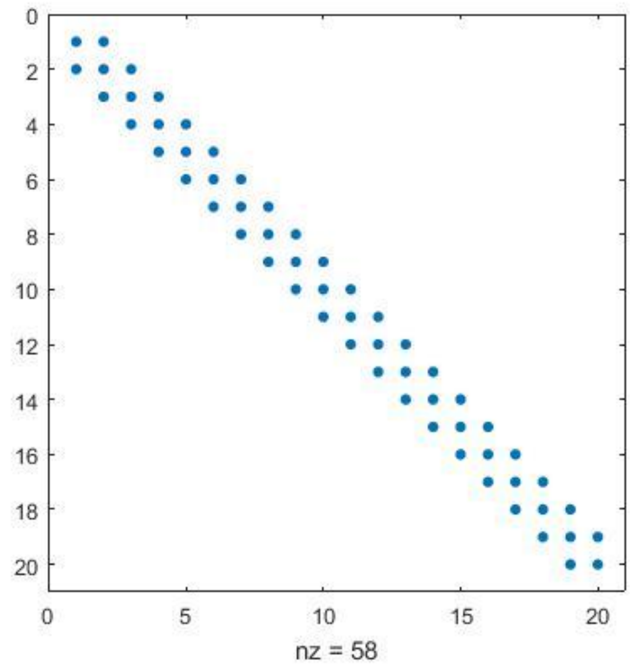
Space Nodes	T_{max} [After 1 year]	% difference
5	300.77	0.063
40	300.96	
80	300.94	0.00
160	300.94	
200	300.94	0.006
250	300.92	
300	300.93	0.00
400	300.93	
600	300.93	0.00
800	300.93	

From the above grid independent test, it seems that the solution is not varying after 300 nodes of space discretization. Therefore, to reduce the computational time there is no need to select more grid points than 300. Therefore, all our solution will be computed by selecting 300 grid points.

2.4.2 Computational Time

Computational time for the solver to compute the solution is 0.567404 seconds

2.4.3 Structure of a Matrix "A"



The structure of a Matrix A is banded matrix with a bandwidth of 3. Therefore, this matrix can be solving with the help of tridiagonal solver (Thomas algorithm).

2.4.4 Accuracy

Temperature distribution is computed using Backward Euler method which has accuracy of single derivative in O (Δt) in time and second order in space O$(\Delta x)^2$. The accuracy of matrix A is computed using condition number and it is found to be 345 which is not high enough. Therefore, the matrix "A" is not ill-conditioned.

2.4.5 Cost of computing

The matrix "A" is compactly banded and having a bandwidth of 3 therefore it is tridiagonal system and can be solved by Thomas algorithm in which total arithmetic operations are of the order of O(N). I have solved this system of equation by using MATLAB "backslash" operator and tridiagonal algorithm is implemented by backslash operator after looking at the structure of the matrix. The cost of computing for Thomas algorithm is 0.51 seconds.

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3. MATLAB Solver

3. 1 PdEPE solver

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right) = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right)$$

The matlab solver uses the above eqaution to solve the partial differential eqations. This equation is compared with our main partial differential equation. By comparing, we can evaluate the value of m that is 2 for cylinderical co-ordinates and 1 for cartesian co-ordinates. So, for PDEfun we can extract data like as mentioned below:

m = 2

c=1/k

f = dudx

s = ${T_{rod}}^{e^{-t/\tau_o}}\Big/_{a^2}$ Source term

for boundary condition, we must make it in form like mentioned below:

$$p(x,t,u) + q(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0$$

So by comparing with the above equation we can extract the boundary conditions as mentioned in the boundary function.

Initial condition is staright forward and we have to make an function to call intial condition that is at 300 k temperature.

Main Program for PDEPE Solver

```
clc; clear; format long e;
k=2*10^7;   % Thermal Conductivity of the Nuclear waste rod
ub=300;
ua=1;
xL=0;
xR=100;     %effected radius
u0=300;
uR=300;
u_rod=1;
t0=0;
tfinal=10;
t=linspace(t0,tfinal,101);
```

```
x=linspace(xL,xR,25);
tic
sol=pdepe(2,@pdefun2,@pdeic2,@pdebc2,x,t,[],k,u0,ua,ub);
for jj =1:1:length(t)
    plot(x,sol(jj,:),'-d');
    title('PDEPE Function');
end
toc
surfc(x,t,sol);
```

PDE function:

```
function [c,f,s] = pdefun2(u,t,T,DuDx,k,u0,ua,ub)
c=1/k;
f=DuDx;
s=(exp(-t/100))/(25)^2;
```

Boundary Condition function

```
function [pL,qL,pR,qR] = pdebc2(xL,uL,xR,uR,t,k,u0,ua,ub)
pL=0;
qL=1;
pR=uR-ub;
qR=0;
```

Initial Boundary Condition

```
function u01=pdeic2(x,k,u0,ua,ub)
u01=300;
```

3.2 Comparison of cost of computing for backward Euler method and PDEPE solver

Method	Computational Cost
Backward Euler Method(Implicit)	0.51 Seconds
PDEPE Solver	2.59 Seconds

4. Result and Discussion

The problem involves the study of temperature distribution and variation of temperature of nuclear waste rod with time. Radioactive nuclear rod is modelled to have source term which is like heat generation. It is very critical to find the time for nuclear rod temperature to reach at study state. This physical problem is modelled in 1-D Cylindrical Co-ordinates parabolic equation. As we know that, in parabolic equation, there is a jump in variable in initial time then it will go to study state. So, this study is find the time taken by nuclear rod to reach at steady state. The problem is solved by using two different techniques to measure the temperature distribution with time as shown in *Figure 1, Figure 2, Figure 3* and *Figure 4.*

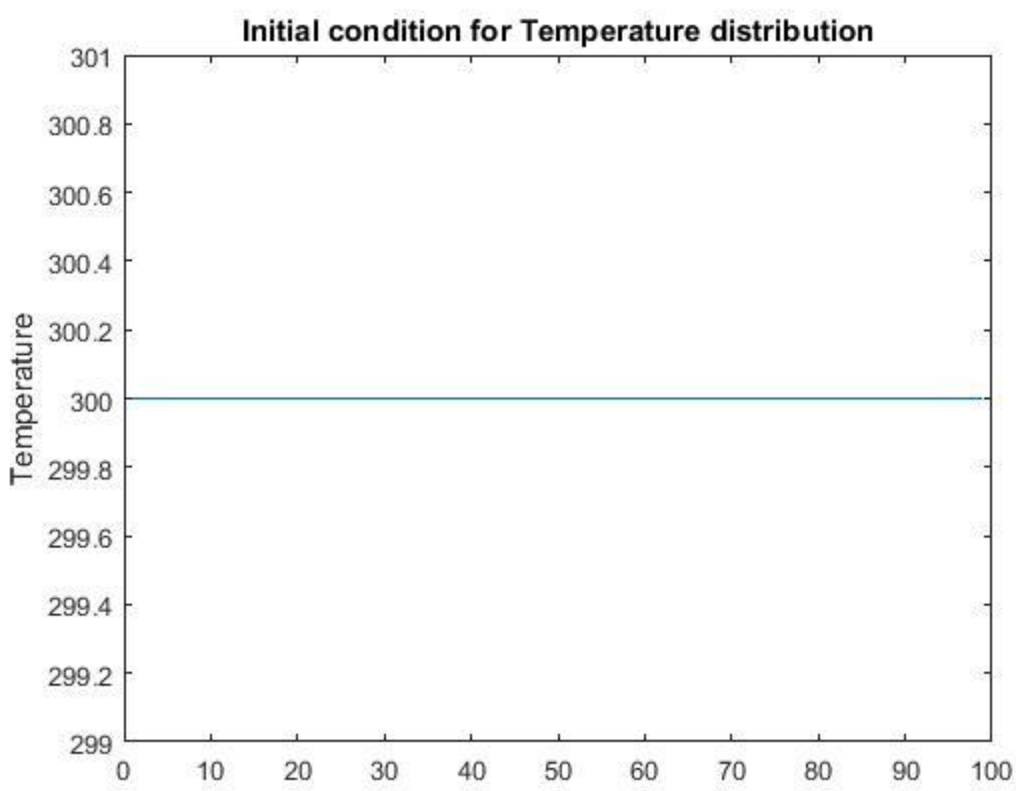

Figure 1 Initial Condition

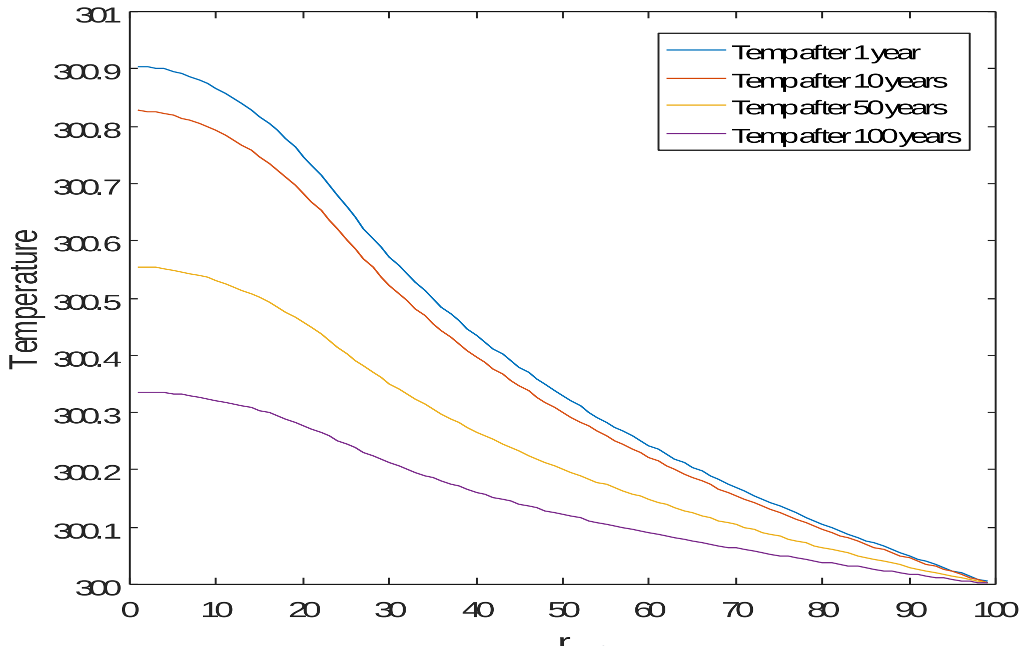

Figure 3 Temperature Variation with Time

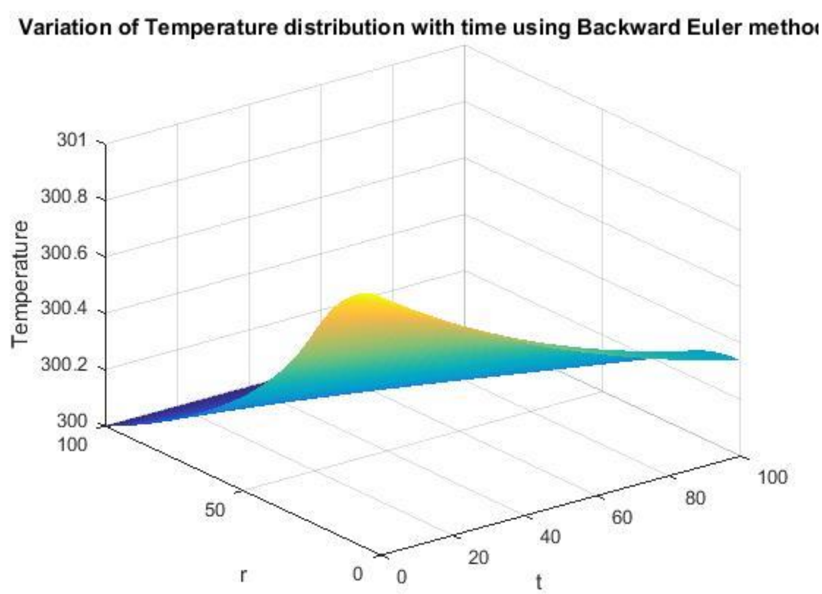

Figure 2 Mesh Plot showing temperature variation with time

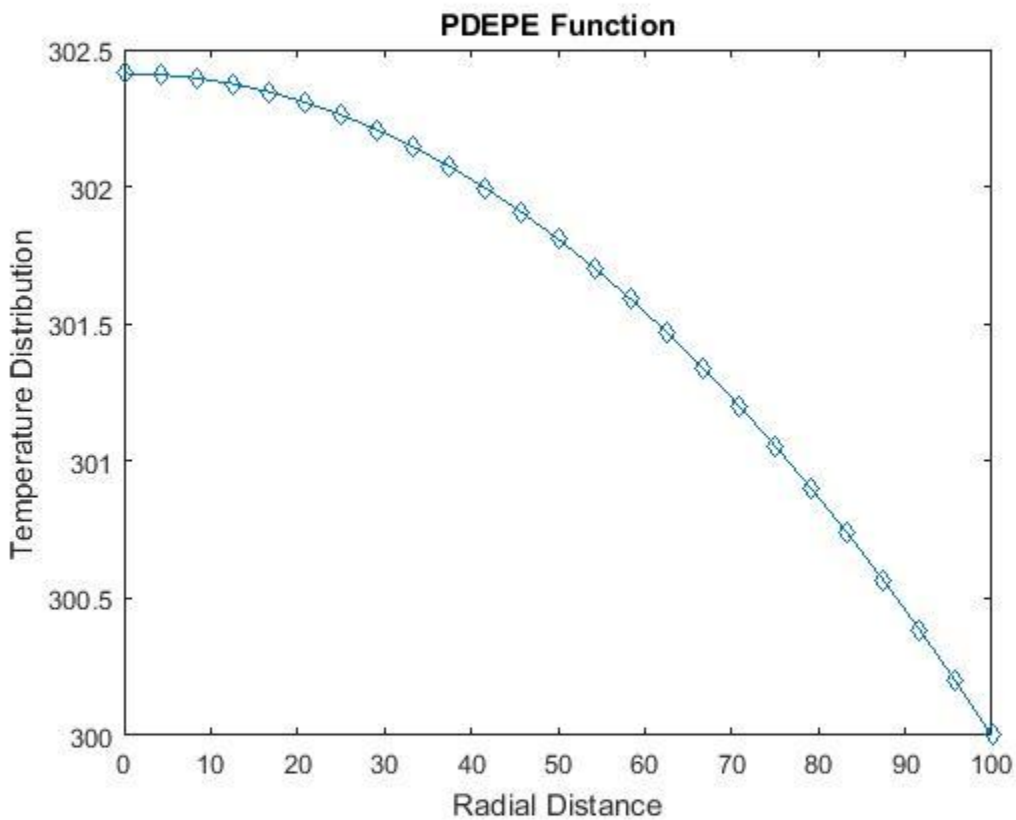

Figure 4 Temperature variation with time PDEPE Solver

Reference:

[1] Ozisik Necati M.,"Finite difference methods in heat transfer" Edition 1994,pp. 75-138.

[2] Lecture Notes" Hand written notes for partial differential equation" Prof. Hossain (The University of western Ontario)

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