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Nuclear, Plasma & Radiological Engineering Department

CP01

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1. PROBLEM DEFINITION

1.1 Formulation

1.1.1 Domain

$$0 \leq r \leq R$$

1.1.2 PDE

$$\frac{1}{\alpha} \frac{\partial T(r, t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T(r, t)}{\partial r} \right)$$

1.1.3 Boundary Conditions

$$\lim_{r \rightarrow 0} T(r, t) \neq \pm \infty$$

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=R} = 0$$

1.1.4 Initial Condition

$$T(r, 0) = \frac{T_0}{2} \left(1 - \cos\left(\frac{\pi r}{R}\right) \right)$$

1.2 Data

Table 1 shows the problem parameters.

Table 1 Problem Parameters

Parameter	Value	Unit
R	3	cm
k	15	W m ⁻¹ K ⁻¹
ρ	8000	Kg m ⁻³
c _p	500	J kg ⁻¹ K ⁻¹
T ₀	500	°C

2. ANALYTICAL SOLUTION

2.1 Steady State Temperature (T_{ss})

The sphere is insulated and symmetric so the steady state temperature will be a constant value. Since the sphere is insulated, the internal energy of the sphere will not change as the temperature profile develops

$$\Delta U = 0$$

$$mc(T_{ss} - \bar{T}_i) = 0$$

$$T_{ss} = \bar{T}_i = \frac{1}{V} \int_0^R T_i dr = \frac{3T_0}{2R^3} \int_0^R r^2 \left(1 - \cos\left(\frac{\pi r}{R}\right)\right) dr$$

Carrying the integration yields

$$T_{ss} = \left(\frac{1}{2} + \frac{3}{\pi^2}\right) T_0$$

2.2 Temperature Distribution Sketch

Figure 1 shows the sketch of the temperature distribution at 6 different time stamps: $t_0 < t_1 < t_2 < t_3 < t_4 < t_\infty$.

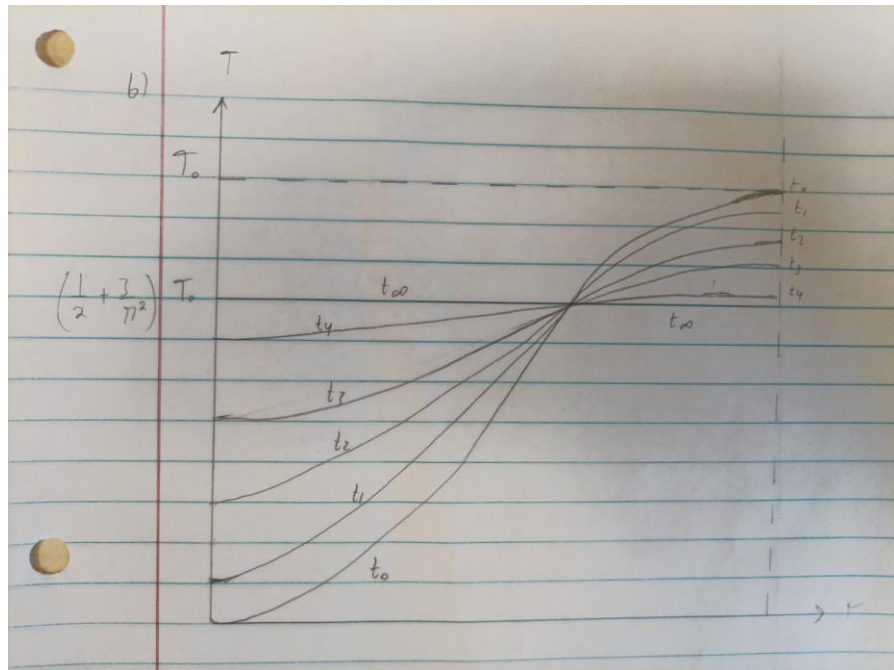


Figure 1 Temperature distribution sketch at six different timestamps

2.3 Time Dependent Temperature Distribution (T(r,t))

$$\text{Let } u(r, t) = r T(r, t)$$

The new formulation of the PDE in terms of $u(r, t)$ becomes

$$\frac{1}{\alpha} \frac{\partial u(r, t)}{\partial t} = \frac{\partial^2 u(r, t)}{\partial r^2}$$

and the boundary conditions become

$$\lim_{r \rightarrow 0} \frac{u(r, t)}{r} \neq \pm \infty$$

$$\left. \frac{\partial u(r, t)}{\partial r} \right|_{r=R} - \frac{u(R, t)}{R} = 0$$

Note that there is no need to transform the initial condition in terms of u because it will be applied at the end of the solution in terms of T . The PDE and the boundary conditions are homogenous so the problem could be solved with the separation of variables.

$$\text{Let } u(r, T) = \psi(r) \Gamma(t)$$

Substitute in the PDE

$$\frac{\psi(r)}{\alpha} \frac{d\Gamma(t)}{dt} = \frac{\Gamma(t) d^2\psi(r)}{dr^2}$$

Divide both sides by $\psi(r) \Gamma(t)$

$$\frac{1}{\alpha \Gamma(t)} \frac{d\Gamma(t)}{dt} = \frac{1}{\psi(r)} \frac{d^2\psi(r)}{dr^2} = -\lambda^2$$

Where λ is a constant

The formulation of the $\psi(r)$ problem becomes

$$\frac{d^2\psi(r)}{dr^2} + \lambda^2 \psi(r) = 0$$

with boundary conditions

$$\lim_{r \rightarrow 0} \frac{\psi(r, t)}{r} \neq \pm \infty$$

$$\frac{d\psi(r, t)}{dr} \Big|_{r=R} - \frac{\psi(R, t)}{R} = 0$$

The solution of the differential equation yields the eigenfunction

$$\psi(r) = c_1 \sin(\lambda r) + c_2 \cos(\lambda r)$$

Applying the boundary condition at $r = 0$

$$\begin{aligned} \lim_{r \rightarrow 0} \frac{\psi(r, t)}{r} &\neq \pm \infty \\ \lim_{r \rightarrow 0} \left(\frac{c_1 \sin(\lambda r)}{r} + \frac{c_2 \sin(\lambda r)}{r} \right) &\neq \pm \infty \\ \lim_{r \rightarrow 0} \frac{c_1 \sin(\lambda r)}{r} + \lim_{r \rightarrow 0} \frac{c_2 \cos(\lambda r)}{r} &\neq \pm \infty \\ c_1 \lambda + \lim_{r \rightarrow 0} \frac{c_2}{0} &\neq \pm \infty \end{aligned}$$

The condition will not be satisfied unless $c_2 = 0$.

$$\psi(r) = c_1 \sin(\lambda r)$$

Applying the boundary condition at $r = R$

$$\begin{aligned} \frac{d\psi(r, t)}{dr} \Big|_{r=R} - \frac{\psi(R, t)}{R} &= 0 \\ c_1 \lambda \cos(\lambda R) - \frac{c_1 \sin(\lambda R)}{R} &= 0 \end{aligned}$$

Multiply both sides by $\frac{-R}{c_1 \cos(\lambda R)}$ and adding the subscript n to λ yields the transcendental eigenvalue equation

$$\tan(\lambda_n R) - \lambda_n R = 0$$

Where $n = 1, 2, 3, \dots, \infty$.

The equation could be solved numerically to obtain the eigenvalues. Note that $\lambda = 0$ is also a solution to the transcendental equation which will yield a different eigenfunction corresponding to the steady state solution. Since the steady state solution have been evaluated already, we will ignore that case from our solution until we transform the problem back in terms of T .

The formulation of the $\Gamma(t)$ problem becomes

$$\frac{d\Gamma(t)}{dt} + \alpha\lambda^2\Gamma(t) = 0$$

The solution of the differential equation yields

$$\Gamma(t) = c_3 e^{-\alpha\lambda^2 t}$$

Substituting the expressions for $\Gamma(t)$ and $\psi(r)$ into $u(r, t)$ while ignoring the $\lambda = 0$ case yields

$$u(r, t) = \sum_{n=1}^{\infty} c_n \sin(\lambda_n r) e^{-\alpha\lambda_n^2 t}$$

Transforming the solution in terms of $T(r, t)$ and including the steady state solution yields

$$T(r, t) = T_{ss} + \sum_{n=1}^{\infty} c_n \frac{\sin(\lambda_n r)}{r} e^{-\alpha\lambda_n^2 t}$$

Apply the initial condition

$$T(r, 0) = \frac{T_0}{2} \left(1 - \cos\left(\frac{\pi r}{R}\right)\right)$$

$$\frac{T_0}{2} \left(1 - \cos\left(\frac{\pi r}{R}\right)\right) = T_{ss} + \sum_{n=1}^{\infty} c_n \frac{\sin(\lambda_n r)}{r}$$

Operating on both sides by $\int_0^R r \sin(\lambda_m r) dr$

$$\int_0^R r \sin(\lambda_m r) \frac{T_0}{2} \left(1 - \cos\left(\frac{\pi r}{R}\right)\right) dr = T_{ss} \int_0^R r \sin(\lambda_m r) dr + \sum_{n=1}^{\infty} c_n \int_0^R \sin(\lambda_m r) \sin(\lambda_n r) dr$$

Due to orthogonality of eigenfunctions

$$\int_0^R r \sin(\lambda_m r) dr = 0$$

and

$$\int_0^R \sin(\lambda_m r) \sin(\lambda_n r) dr = 0 \text{ for } n \neq m$$

The equation becomes

$$c_n = \frac{\frac{T_0}{2} \int_0^R r \sin(\lambda_n r) \left(1 - \cos\left(\frac{\pi r}{R}\right)\right) dr}{\int_0^R \sin(\lambda_n r)^2 dr}$$

The final solution becomes

$$T(r, t) = T_{ss} + \sum_{n=1}^{\infty} c_n \frac{\sin(\lambda_n r)}{r} e^{-\alpha \lambda_n^2 t}$$

where

$$T_{ss} = \left(\frac{1}{2} + \frac{3}{\pi^2}\right) T_0$$

and

$$c_n = \frac{\frac{T_0}{2} \int_0^R r \sin(\lambda_n r) \left(1 - \cos\left(\frac{\pi r}{R}\right)\right) dr}{\int_0^R \sin(\lambda_n r)^2 dr}$$

2.4 Eigenvalue Evaluation

To evaluate the analytical temperature, we need to solve the eigenvalues equation to obtain the eigenvalues then evaluate c_n . Since the eigenvalue equation is transcendental, it will be solved numerically. We first plot the eigenvalue equation (see Figure 2) to estimate good initial guesses for the numerical solver to decrease the number of iterations required. After that, the eigenvalues equation is solved numerically to obtain the eigenvalues. The values of c_n are computed for the first 10 eigenvalues. Table 2 shows the first 10 eigenvalues and corresponding c_n .

Table 2 First 10 eigenvalues and corresponding c value

n	λ_n	c_n
1	1.49780315263635E+02	-2.84750138890469E+00
2	2.57508394564590E+02	+1.20336636097018E-01
3	3.63470721980963E+02	-2.50118337276080E-02
4	4.68873130427711E+02	+8.39952093726840E-03
5	5.74025175731002E+02	-3.60863240293182E-03
6	6.79043431976234E+02	+1.80623996540356E-03
7	7.83981749956298E+02	-1.00401850548188E-03
8	8.88868475293755E+02	+6.02603141315715E-04
9	9.93719959696431E+02	-3.83551779972611E-04
10	1.09854630132743E+03	+2.55735666255434E-04

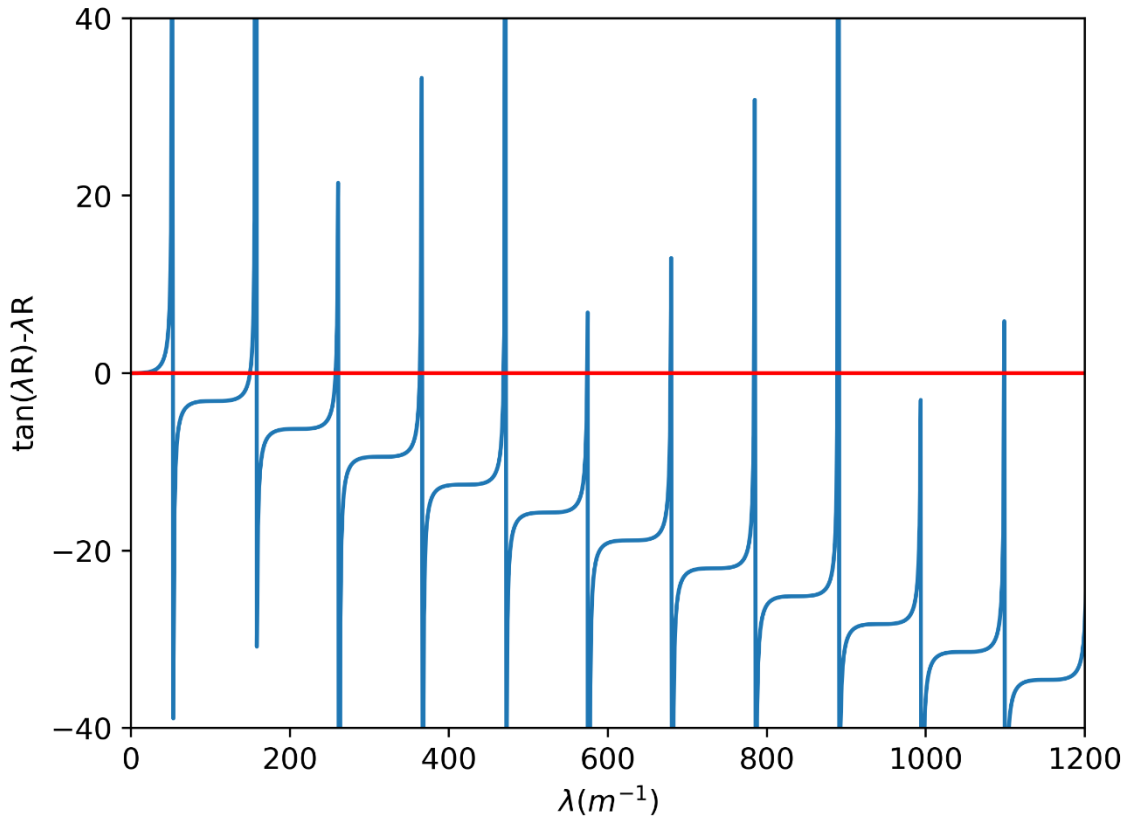


Figure 2 Eigenvalues equation plot

2.5 Convergence

To estimate the number of terms required to achieve good convergence, the following procedure was applied: 7 timestamps (0s, 5s, 10s, 15s, 20s, 40s, 60s) were chosen to capture the time evolution of the temperature distribution. The domain was divided into 100 equally sized elements. For each timestamp the temperature distribution was evaluated for increasing number of terms in the series. The following equation was used to assess the convergence

$$\epsilon_{jn} = \max_{i=0}^I \left| \frac{T(r_i, t_j)_n - T(r_i, t_j)_{n-1}}{T(r_i, t_j)_{n-1}} \right|$$

where i is the space index, j is the timestamp index and n is the number of terms taken from the series. The results are summarized in Table 3 for the first 5 terms in the series. Also Figure 3 shows the temperature distribution for different number of terms for the seven timestamps. We can see from Table 3 that the ϵ is decreasing as n increases for all timestamps except at $t = 0$ it is alternating. It is evident from Table 3 and Figure 3 that 5 terms are enough to achieve excellent convergence for all timestamps except the initial temperature which can be evaluated directly from the initial condition. Figure 4 shows the converged analytical temperature distribution at the 7 timestamps.

Table 3 Convergence assessment

n	t = 0	t = 5s	t = 10s	t = 15s	t = 20s	t = 40s	t = 60s
1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
2	N/A	7.E-02	1.E-02	3.E-03	7.E-04	4.E-06	3.E-08
3	1.E+00	6.E-03	3.E-04	2.E-05	1.E-06	6.E-11	3.E-15
4	7.E+00	5.E-04	5.E-06	6.E-08	8.E-10	1.E-16	5.E-17
5	2.E+00	3.E-05	4.E-08	7.E-11	1.E-13	5.E-17	5.E-17

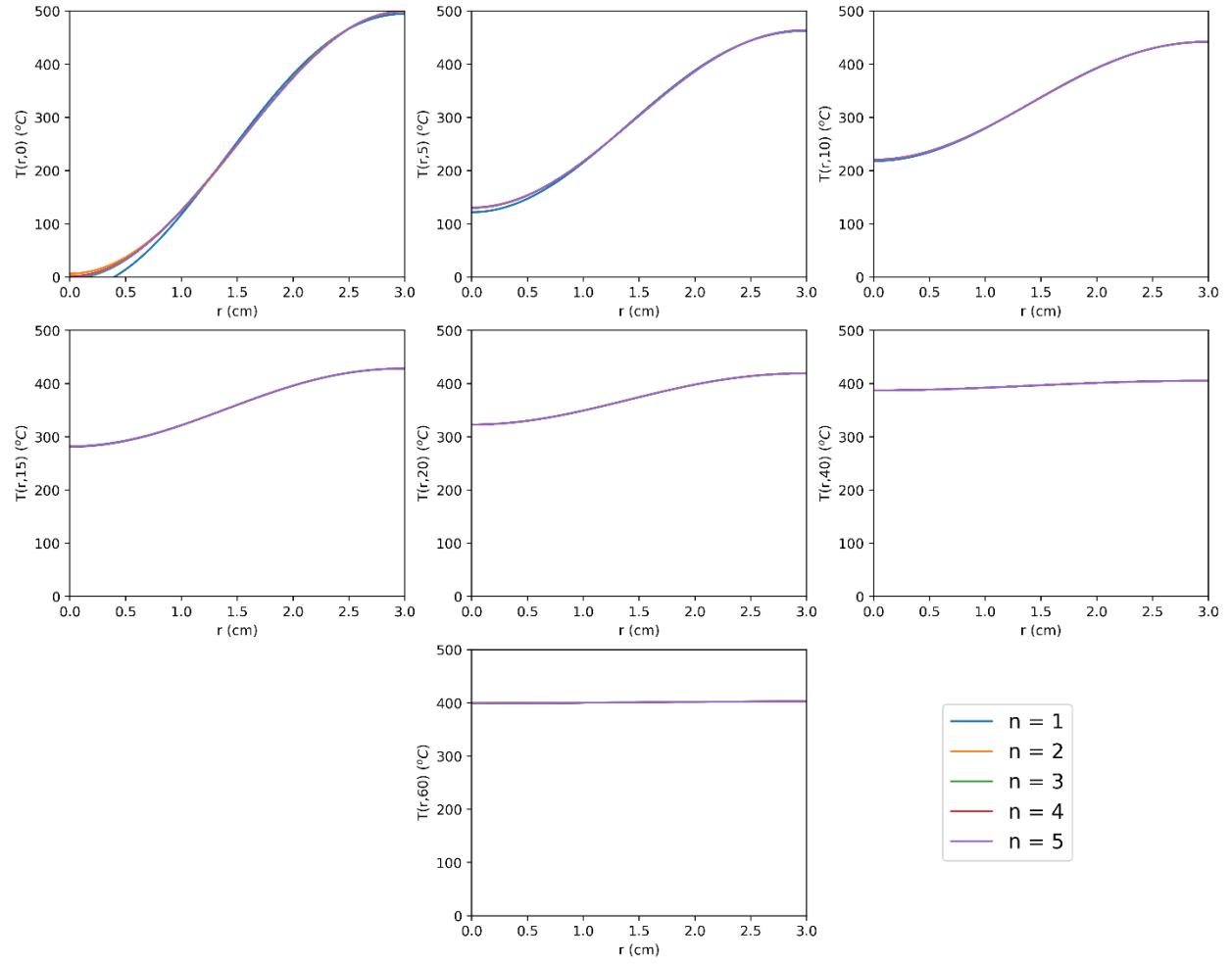


Figure 3 Analytical temperature distribution at 7 different timestamps for an increasing number of terms in the series

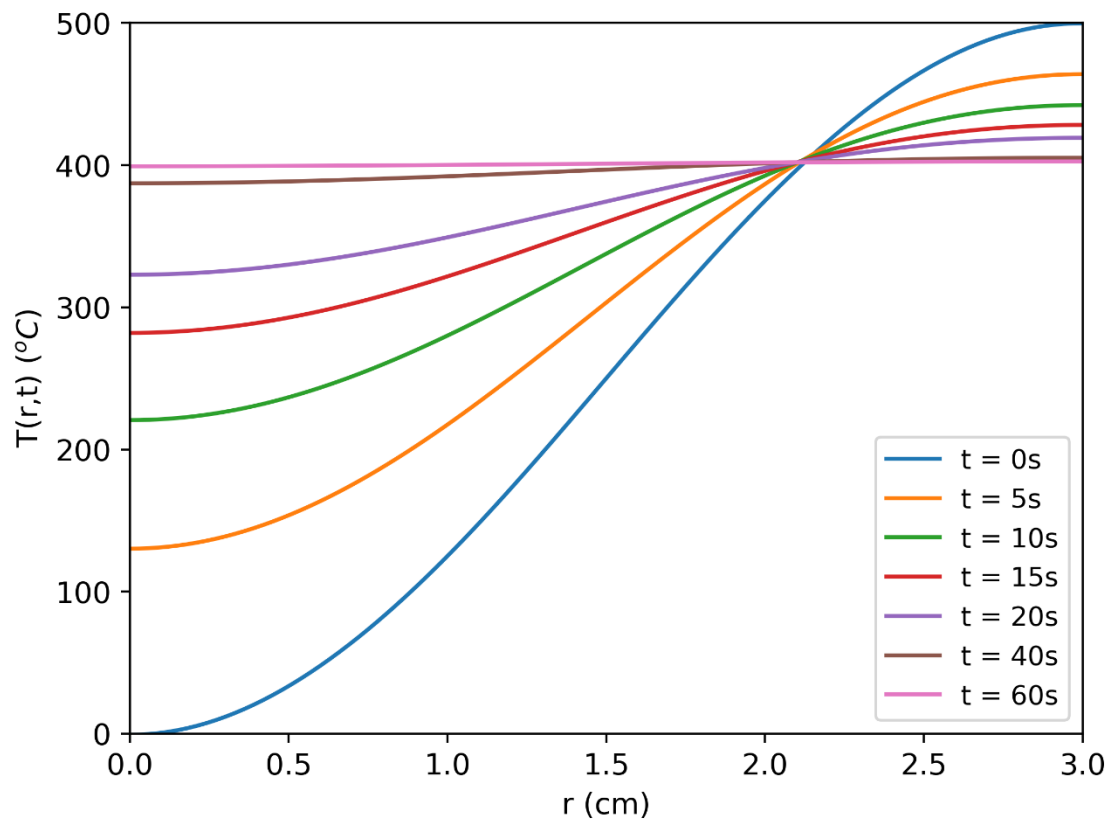


Figure 4 Analytical Temperature Distribution

3. NUMERICAL SOLUTION

3.1 Finite Difference Formulation

First the domain was divided into $I+1$ equally spaced nodes as shown in Figure 5. The mesh size is defined as

$$\Delta r = r_i - r_{i-1} = \frac{R}{I}$$

The time axis was divided into equally spaced $J + 1$ time instances between 0 and 60 as shown in Figure 6. The times step is defined as

$$\Delta t = t_j - t_{j-1} = \frac{60}{J}$$

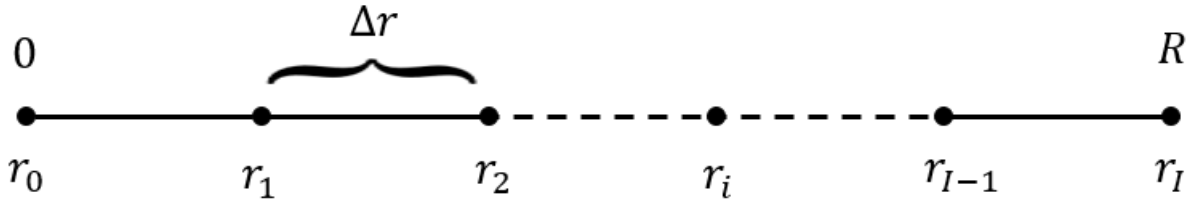


Figure 5 Mesh

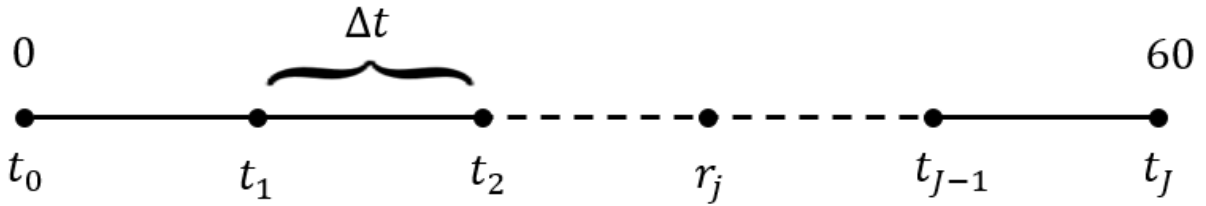


Figure 6 Time Axis Discretization

The central finite difference second order approximation for the first space derivative of the temperature is defined as

$$\frac{\partial T(r, t)}{\partial r} \Big|_i^j = \frac{T_{i+1}^j - T_{i-1}^j}{2\Delta r}$$

Then the second space derivative of the temperature becomes

$$\frac{\partial^2 T(r, t)}{\partial r^2} \Big|_i^j = \frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{\Delta r^2}$$

The forward first order finite difference approximation for the time derivative of the temperature is defined as

$$\frac{\partial T(r, t)}{\partial t} \Big|_i^j = \frac{T_i^{j+1} - T_i^j}{\Delta t}$$

Substituting these equations into the PDE and rearranging yields

$$T_i^{j+1} = T_i^j + \frac{\alpha \Delta t}{\Delta r^2} (T_{i+1}^j - 2T_i^j + T_{i-1}^j) + \frac{\alpha \Delta t}{r \Delta r} (T_{i+1}^j - T_{i-1}^j)$$

This equation can be used to compute the temperature at any interior node at any time instance. The first boundary condition could be written as

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

If the temperature at a fictitious node outside the domain with distance Δr from the left of node r_0 is T_{-1}^j then the boundary condition could be written as.

$$\frac{\partial T(r, t)}{\partial r} \Big|_0^j = \frac{T_1^j - T_{-1}^j}{2\Delta r} = 0$$

Which gives

$$T_{-1}^j = T_1^j$$

Substituting into the finite difference equation of node 0 yields

$$T_0^{j+1} = T_0^j + \frac{2\alpha \Delta t}{\Delta r^2} (T_1^j - T_0^j)$$

And similarly, the second boundary condition becomes

$$T_I^{j+1} = T_I^j + \frac{2\alpha \Delta t}{\Delta r^2} (T_{I-1}^j - T_I^j)$$

To find the values of the temperatures, the finite difference equation is applied at each time instance for all nodes.

3.2 Mesh Refinement Study

A mesh refinement study was conducted by evaluating the numerical temperature at the seven timestamps for decreasingly mesh size. We started with a mesh size of 3×2^{-1} cm and then reduced the mesh size by a factor of 2 each iteration. Figure 7 shows the results of this study. It is obvious that solution accuracy become independent of the mesh size starting from mesh size 3×2^{-4} cm. To achieve better smoothness in the solution and to avoid unnecessary increase in the computational time we chose the mesh size to be 3×2^{-5} cm in the time step study and in the final evaluation of the numerical temperature.

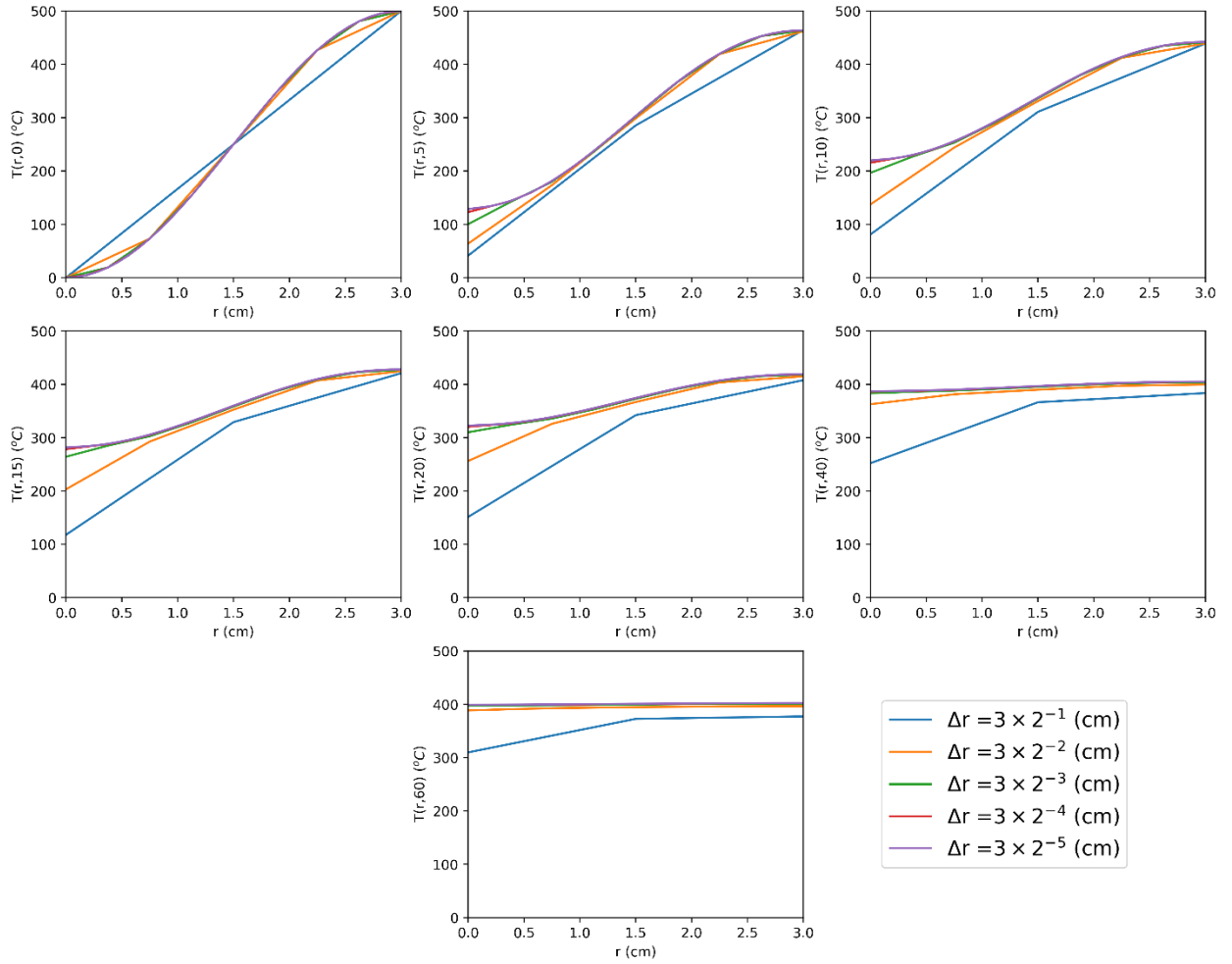


Figure 7 Temperature distribution at the seven timestamps for different mesh sizes

3.3 Time Step Study

It can be shown that to achieve convergence and stability in the results of the finite difference solution the following condition must be satisfied [1]

$$\Delta t \leq \frac{1}{2} \frac{\Delta r^2}{\alpha}$$

Substituting our final mesh size $\Delta r = 3 \times 2^{-5} \text{ cm} = 0.03 \times 2^{-5} \text{ m}$ into the inequality yields

$$\Delta t \leq 0.12 \text{ s}$$

And To avoid oscillation of errors, it is recommended to choose Δt less than half this value [1]. To explore this relation, we performed a time step study with 3 different values for the time step (0.2, 0.1, 0.05). Figure 8 shows that the solution didn't achieve convergence with time step 0.2s as expected. On the other hand, Figure 9 shows that the solution achieved convergence for both time steps 0.1s and 0.05s. To avoid oscillating errors and unnecessary computation time, we chose the time step to be 0.05s in our final evaluation.

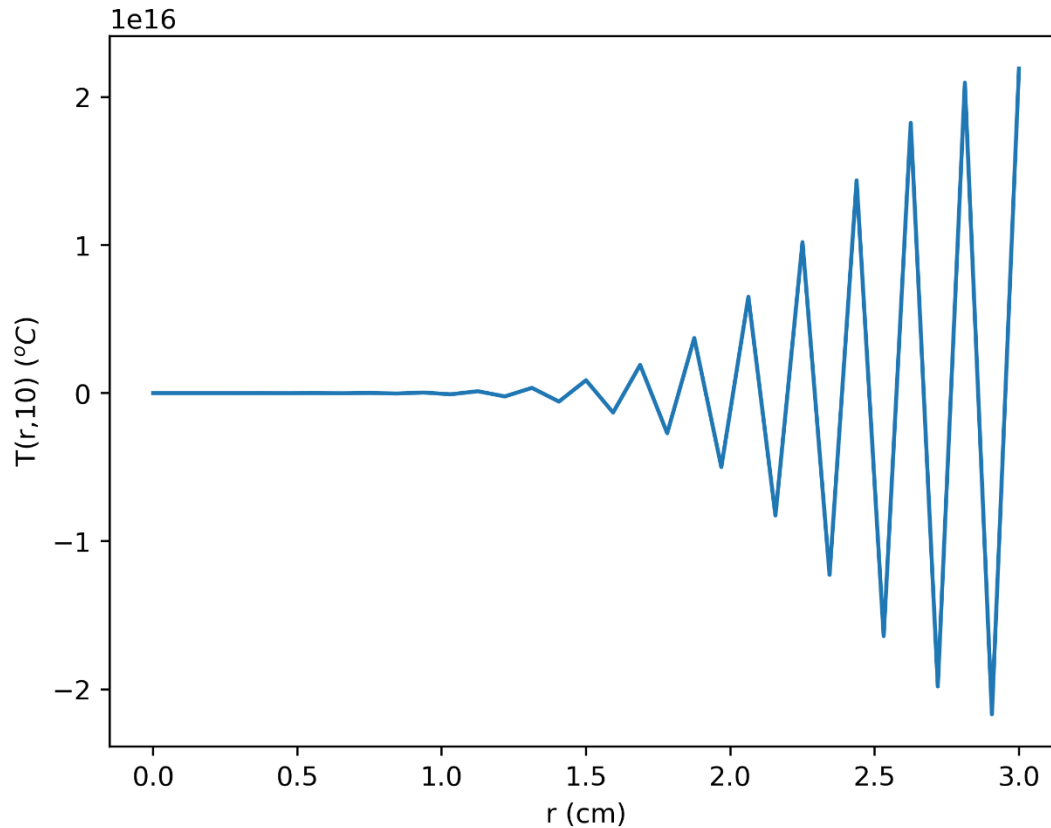


Figure 8 Non Converged Temperature distribution at time = 10 s and $\Delta t = 0.2 \text{ s}$

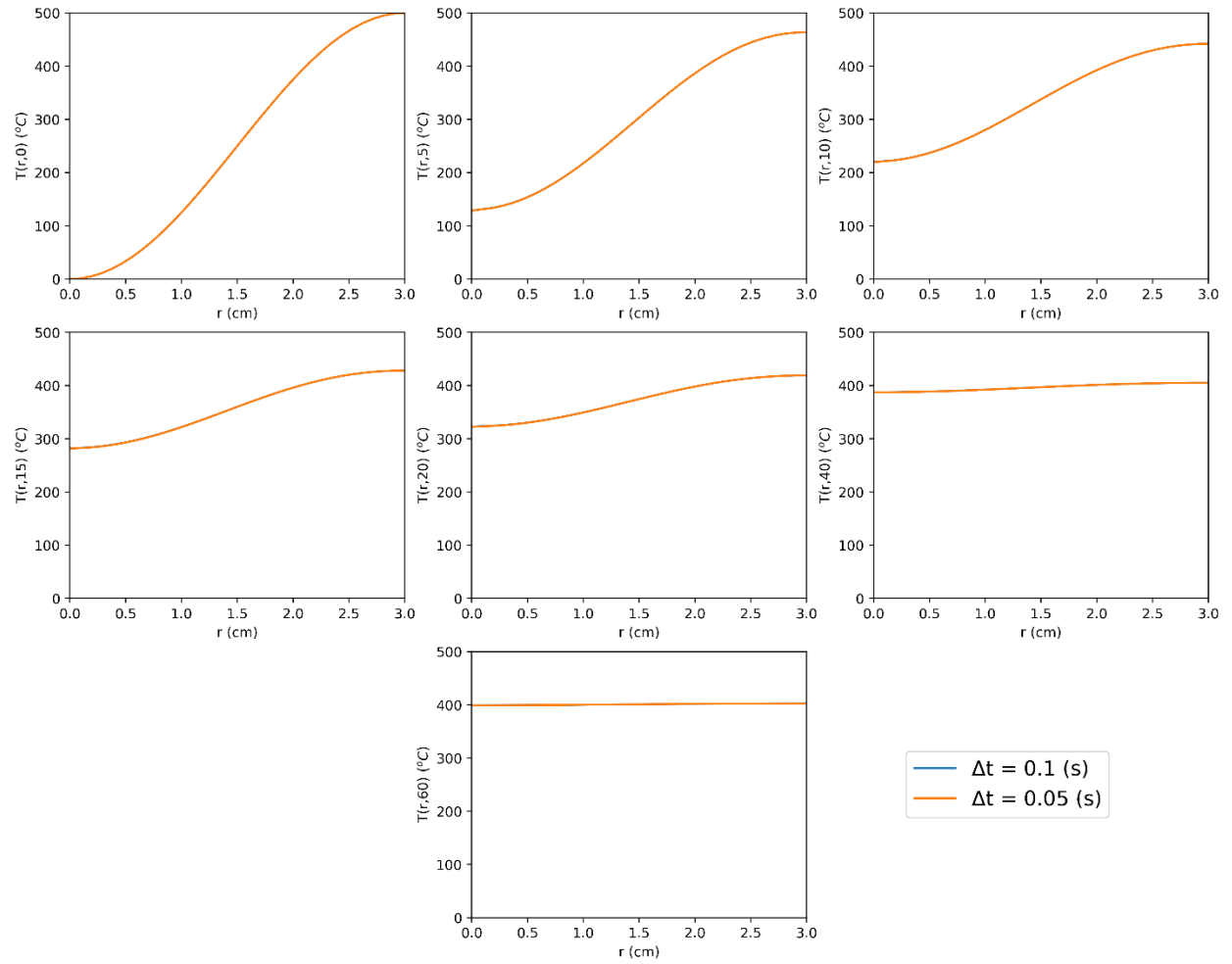


Figure 9 Temperature distribution at seven different timestamps for two different time steps

3.4 Numerical and Analytical Solutions Comparison

Figure 10 shows the comparison between the converged analytical and numerical solutions. It is clear from the figure that the two solutions match exactly.

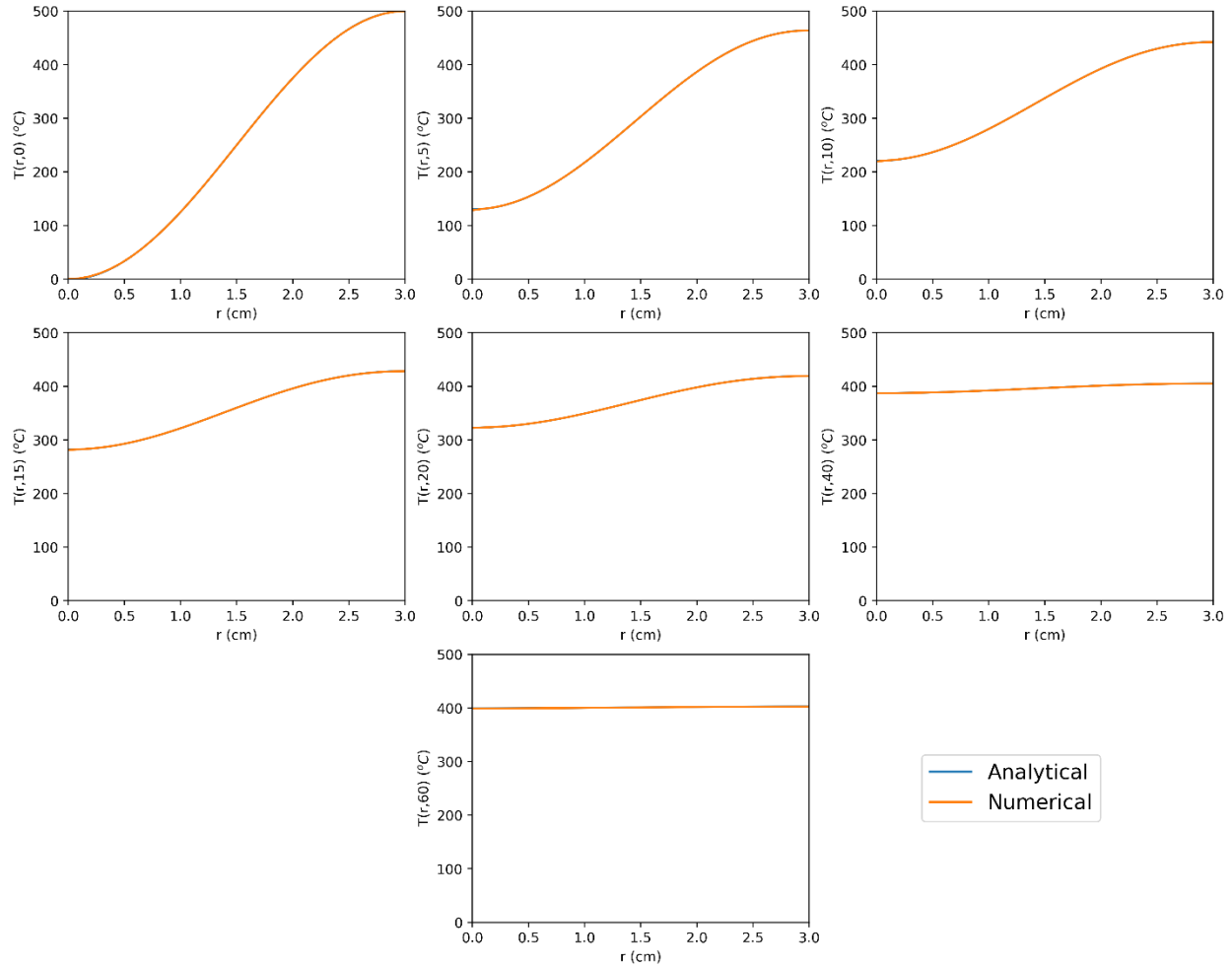


Figure 10 Converged analytical and numerical temperature distributions at seven different timestamps

4. CONCLUSION

The aim of this study was to solve a 1D time dependent heat conduction problem in spherical coordinates using the finite difference method. The problem was first solved analytically, and a study was made to assess the number of terms required from the series to achieve convergence. A suitable number of terms was found to be 5. The finite difference method was implemented in a python code. A grid refinement study was done and the mesh size chosen was 3×2^{-5} cm which corresponds to 32 elements in the domain. Another study was made to find a reasonable time step that achieves convergence without error oscillation and it was found to be 0.05 s. Finally the analytical and numerical solutions were compared and the difference between them was found to be negligible.

5. REFERENCES

- [1] S. C. Chapra, R. P. Canale, *Numerical Methods for Engineers*, 7th ed. New York: McGraw-Hill Education, 2015.

APPENDIX

https://github.com/MohamedElkamash/finite_diff

This is the link of the Github repository of the project. The repository contains all the code files and the results including csv files and the figures in this report. I didn't put the code here because it consists of multiple files.