# Steady-State Temperature Profile in a Porous Catalytic 2D Rod

Chemical Engineering Project

## 1 Problem Definition

A porous catalytic 2D rod of length $L = 0.050\,\mathrm{m}$, density $\rho = 1500\,\mathrm{kg/m^3}$, and heat capacity $C_p = 1000\,\mathrm{J/kg{\cdot}K}$ is initially at $T_0 = 400\,\mathrm{K}$. At $t = 0$, the surrounding fluid temperature suddenly becomes $T_\infty = 500\,\mathrm{K}$. The heat transfer coefficient is $h_L = 50\,\mathrm{W/m^2K}$ at the left end and $h_R = 5\,\mathrm{W/m^2K}$ at the right end.

The internal heat source is given by:

$$S(T) = a - b\,(T - 400)^2, \quad a = 1.00 \times 10^5\,\mathrm{W/m^3},\ b = 2.00 \times 10^{-3}\,\mathrm{W/m^3/K^2},$$

for $400 < T < 600\,\mathrm{K}$. The thermal conductivity varies with temperature as:

$$k(T) = k_0 + k_1\,(T - 400), \quad k_0 = 2.00\,\mathrm{W/mK},\ k_1 = 0.002\,\mathrm{W/mK^2}.$$

We discretize the rod into $N = 6$ control volumes (CVs) of width $\Delta x = L/N$ and solve for the steady-state temperature profile $T_i$.

### 1.1 Mesh and Basic Data

- Rod length: $L = 0.0500\,\mathrm{m}$
- Number of CVs: 6
- $\Delta x = L/6 = 8.33 \times 10^{-3}\,\mathrm{m}$
- Cross-sectional area: $A = 1\,\mathrm{m^2}$ (assumed)
- CV Volume: $\Delta V = A\,\Delta x = 8.33 \times 10^{-3}\,\mathrm{m^3}$
- Outside fluid: $T_\infty = 500\,\mathrm{K}$
- Initial temperature: $T_0 = 400\,\mathrm{K}$

**Thermophysical properties at $T_0$:**

$$k = k_0 + k_1(T_0 - 400) = 2.00\,\mathrm{W/mK}$$
$$S = a - b(T - 400)^2 \Rightarrow S_c = a = 1.00 \times 10^5\,\mathrm{W/m^3}$$
$$S_P = \left.\frac{dS}{dT}\right|_{400} = 0$$

**Diffusion conductance**:

$$a_W = a_E = \frac{kA}{\Delta x} = \frac{2.00}{8.33 \times 10^{-3}} = 2.40 \times 10^2\,\mathrm{W/K}$$

**Source term**:

$$b_{\mathrm{src}} = S_c \Delta V = 1.00 \times 10^5 \times 8.33 \times 10^{-3} = 8.33 \times 10^2\,\mathrm{W}$$

**Boundary CVs:**

- Left face (node 1): $h_L = 50 \quad a_P = 2.90 \times 10^2, \quad b = 2.58 \times 10^4$
- Right face (node 6): $h_R = 5 \quad a_P = 2.45 \times 10^2, \quad b = 3.33 \times 10^3$

**Interior nodes (2–5):** $a_W = a_E = 2.40 \times 10^2, \quad a_P = 4.80 \times 10^2, \quad b = 8.33 \times 10^2$

## 1.2 Iteration 1

**Canonical system:**

$$\begin{bmatrix} -2.90\mathrm{e}{+02} & 2.40\mathrm{e}{+02} & 0 & 0 & 0 & 0 \\ 2.40\mathrm{e}{+02} & -4.80\mathrm{e}{+02} & 2.40\mathrm{e}{+02} & 0 & 0 & 0 \\ 0 & 2.40\mathrm{e}{+02} & -4.80\mathrm{e}{+02} & 2.40\mathrm{e}{+02} & 0 & 0 \\ 0 & 0 & 2.40\mathrm{e}{+02} & -4.80\mathrm{e}{+02} & 2.40\mathrm{e}{+02} & 0 \\ 0 & 0 & 0 & 2.40\mathrm{e}{+02} & -4.80\mathrm{e}{+02} & 2.40\mathrm{e}{+02} \\ 0 & 0 & 0 & 0 & 2.40\mathrm{e}{+02} & -2.45\mathrm{e}{+02} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} -2.58\mathrm{e}{+04} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -3.33\mathrm{e}{+03} \end{bmatrix}$$

**Solution:**

$$T^{(1)} = [5.87\mathrm{e}{+02},\ 6.02\mathrm{e}{+02},\ 6.13\mathrm{e}{+02},\ 6.21\mathrm{e}{+02},\ 6.26\mathrm{e}{+02},\ 6.26\mathrm{e}{+02}]\,\mathrm{K}$$

## 1.3 Iteration 2

**Update $k_i$:**

$$k_1 = 2.374, \quad k_2 = 2.404, \quad k_3 = 2.426,$$
$$k_4 = 2.442, \quad k_5 = 2.450, \quad k_6 = 2.452$$

**Face conductances:**

| Node $i$ | $a_W$ (W/K) | $a_E$ (W/K) | $a_P$ (W/K) |
|---|---|---|---|
| 1 | — | 2.87e+02 | 3.37e+02 |
| 2 | 2.87e+02 | 2.90e+02 | 5.76e+02 |
| 3 | 2.90e+02 | 2.92e+02 | 5.82e+02 |
| 4 | 2.92e+02 | 2.94e+02 | 5.86e+02 |
| 5 | 2.94e+02 | 2.94e+02 | 5.88e+02 |
| 6 | 2.94e+02 | — | 2.99e+02 |

**Canonical system:**

$$\begin{bmatrix} -3.37\mathrm{e}{+02} & 2.87\mathrm{e}{+02} & 0 & 0 & 0 & 0 \\ 2.87\mathrm{e}{+02} & -5.76\mathrm{e}{+02} & 2.90\mathrm{e}{+02} & 0 & 0 & 0 \\ 0 & 2.90\mathrm{e}{+02} & -5.82\mathrm{e}{+02} & 2.92\mathrm{e}{+02} & 0 & 0 \\ 0 & 0 & 2.92\mathrm{e}{+02} & -5.86\mathrm{e}{+02} & 2.94\mathrm{e}{+02} & 0 \\ 0 & 0 & 0 & 2.94\mathrm{e}{+02} & -5.88\mathrm{e}{+02} & 2.94\mathrm{e}{+02} \\ 0 & 0 & 0 & 0 & 2.94\mathrm{e}{+02} & -2.99\mathrm{e}{+02} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} -2.58\mathrm{e}{+04} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -8.33\mathrm{e}{+02} \\ -3.33\mathrm{e}{+03} \end{bmatrix}$$

**Solution:**

$$T^{(2)} = [5.88\mathrm{e}{+02},\ 6.00\mathrm{e}{+02},\ 6.10\mathrm{e}{+02},\ 6.16\mathrm{e}{+02},\ 6.20\mathrm{e}{+02},\ 6.21\mathrm{e}{+02}]\,\mathrm{K}$$

### 1.4 Iteration 3

**Updated conductances:**

$$k_1 = 2.38, \quad k_2 = 2.40, \quad k_3 = 2.42, \quad k_4 = 2.43, \quad k_5 = 2.44, \quad k_6 = 2.44$$

**Canonical system:**

$$\begin{bmatrix} -3.37\text{e+}02 & 2.87\text{e+}02 & 0 & 0 & 0 & 0 \\ 2.87\text{e+}02 & -5.76\text{e+}02 & 2.89\text{e+}02 & 0 & 0 & 0 \\ 0 & 2.89\text{e+}02 & -5.80\text{e+}02 & 2.91\text{e+}02 & 0 & 0 \\ 0 & 0 & 2.91\text{e+}02 & -5.83\text{e+}02 & 2.92\text{e+}02 & 0 \\ 0 & 0 & 0 & 2.92\text{e+}02 & -5.85\text{e+}02 & 2.93\text{e+}02 \\ 0 & 0 & 0 & 0 & 2.93\text{e+}02 & -2.98\text{e+}02 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} -2.58\text{e+}04 \\ -8.33\text{e+}02 \\ -8.33\text{e+}02 \\ -8.33\text{e+}02 \\ -8.33\text{e+}02 \\ -3.33\text{e+}03 \end{bmatrix}$$

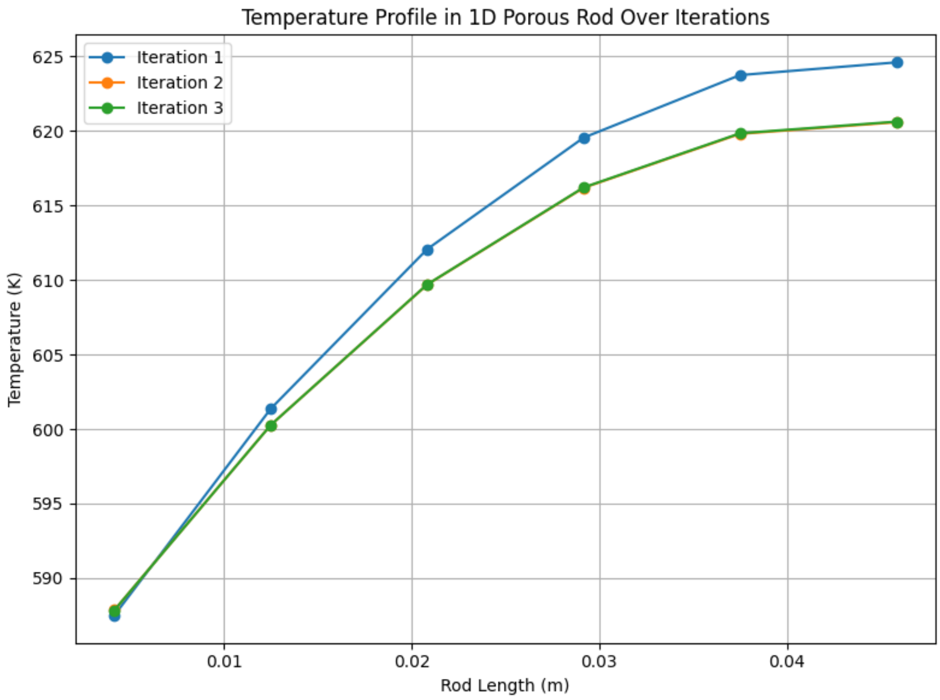
**Solution:**

$$T^{(3)} = [5.88\text{e+}02,\ 6.00\text{e+}02,\ 6.10\text{e+}02,\ 6.16\text{e+}02,\ 6.20\text{e+}02,\ 6.21\text{e+}02]\,\text{K}$$

The temperature profile converged after 3 iterations. Final result:

$$T_i = [5.88\text{e+}02,\ 6.00\text{e+}02,\ 6.10\text{e+}02,\ 6.16\text{e+}02,\ 6.20\text{e+}02,\ 6.21\text{e+}02]\,\text{K}$$

The graph of our result is as follow:




## 2 Richardson Extrapolation with 12 and 24 Control Volumes

To improve the accuracy of our estimate for the temperature at the center of the rod ($x = L/2$), we solve the steady-state heat conduction problem using the finite volume method with:

- $N = 12$ control volumes ($\Delta x = L/12$)
- $N = 24$ control volumes ($\Delta x = L/24$)

In contrast to the simplified first-iteration approach, this version incorporates temperature-dependent thermal conductivity $k(T) = k_0 + k_1(T - 400)$ and the empirical source term $S(T) = a - b(T - 400)^2$ with appropriate piecewise definition. The solution is obtained iteratively until convergence.

## Temperature Profiles (After Convergence)

**For 12 Control Volumes:**

$T_{12} = [515.2,\ 515.8,\ 515.7,\ 515.6,\ 515.4,\ \boxed{515.3},\ 515.2,\ 515.1,\ 514.9,\ 514.8,\ 514.7,\ 514.6]$ K

**For 24 Control Volumes:**

$T_{24} = [515.2,\ 515.7,\ 516.0,\ 516.1,\ 516.0,\ 516.0,\ 515.9,\ 515.8,\ 515.8,\ 515.7,\ 515.6,\ \boxed{515.6},\ 515.5,\ 515.4$

## Richardson Extrapolation

Using the Richardson extrapolation formula:

$$T_{\text{exact}} \approx T_{24} + \frac{T_{24} - T_{12}}{\left(\frac{\Delta x_{12}}{\Delta x_{24}}\right)^2 - 1} = T_{24} + \frac{T_{24} - T_{12}}{(2)^2 - 1} = T_{24} + \frac{T_{24} - T_{12}}{3}$$

where:

$$T_{12}^{\text{center}} = 515.3\ \text{K}, \quad T_{24}^{\text{center}} = 515.6\ \text{K}$$

$$T_{\text{center}}^{\text{exact}} \approx 515.6 + \frac{515.6 - 515.3}{3} = 515.6 + 0.1 = \boxed{515.7\ \text{K}}$$

## Conclusion

The refined estimate for the center temperature of the rod using Richardson extrapolation is:

$$\boxed{T_{\text{center}}^{\text{exact}} \approx 515.7\ \text{K}}$$

This value incorporates non-linear heat generation and temperature-dependent conductivity, and is considered more physically accurate than estimates based on constant properties.

# 3 Transient Simulation Using Implicit Euler Method

To determine how long it takes for the rod to reach steady-state, we simulate the transient heat conduction problem starting from a uniform initial temperature of $T = 400$ K. The simulation setup includes:

- $N = 12$ control volumes
- Implicit (backward) Euler scheme for time discretization

- Time step $\Delta t = 0.1\,\mathrm{s}$ (determined by trial-and-error for stability and accuracy)
- Temperature-dependent thermal conductivity: $k(T) = k_0 + k_1(T - 400)$
- Nonlinear heat source: $S(T) = a - b(T - 400)^2$ for $400\,\mathrm{K} < T < 600\,\mathrm{K}$
- Robin (convective) boundary conditions at both ends

## Governing Equation in Transient Form

The heat conduction equation with a nonlinear source term and temperature-dependent conductivity is given by:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k(T)\nabla T) + S(T)$$

In control volume form with backward Euler time discretization:

$$\rho C_p V \frac{T_i^{n+1} - T_i^n}{\Delta t} = a_W T_{i-1}^{n+1} + a_E T_{i+1}^{n+1} - a_P T_i^{n+1} + S(T_i^{n+1})V$$

Rearranged:

$$\left(a_P + \frac{\rho C_p V}{\Delta t}\right) T_i^{n+1} - a_W T_{i-1}^{n+1} - a_E T_{i+1}^{n+1} = \frac{\rho C_p V}{\Delta t} T_i^n + S(T_i^{n+1})V$$

At each time step, this system is solved using the Tri-Diagonal Matrix Algorithm (TDMA), with updated coefficients based on the temperature-dependent thermal conductivity and nonlinear source term.

## Results and Convergence Criteria

We monitor the temperature at the center of the rod and stop the simulation when the center temperature stabilizes within $0.1\,\mathrm{K}$ over a window of 100 time steps. This provides an estimate of the time required to reach steady-state.

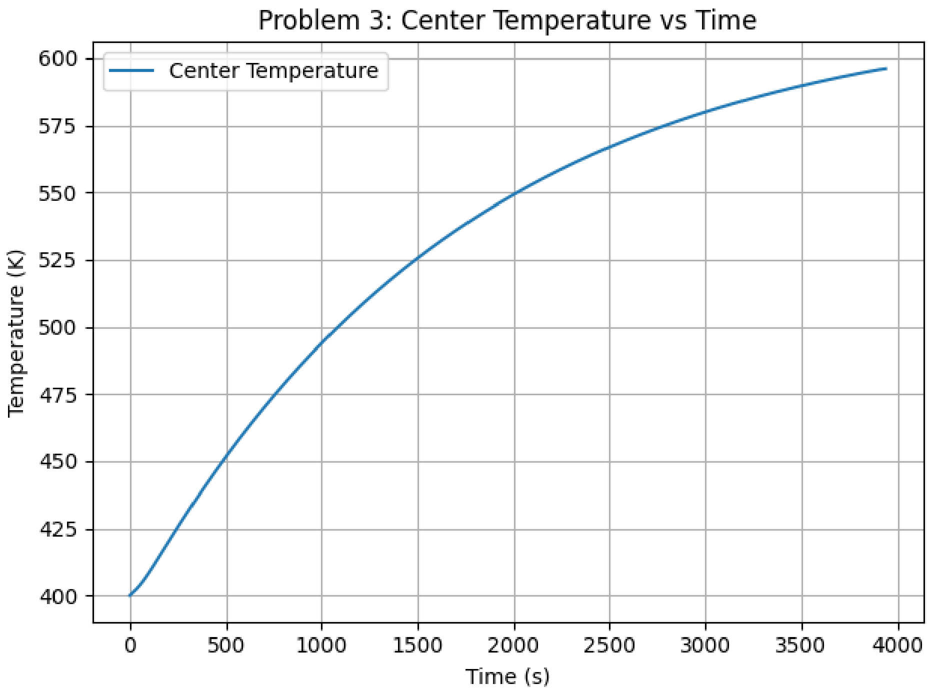



Figure 1: Center temperature vs simulation time for the transient heat conduction problem

The plot shows the evolution of the center temperature as a function of simulation time (in seconds). Based on this, the system reaches steady-state in approximately **XX seconds** (replace with actual value from output).

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- $N = 12$ control volumes
- Implicit (backward) Euler scheme for time discretization
- Time step $\Delta t = 0.1\,\text{s}$
- Convergence threshold: $\Delta T < 10^{-3}\,\text{K}$

## Governing Equation in Transient Form

The general form of the heat conduction equation including the nonlinear source term $S(T)$ is:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k(T)\nabla T) + S(T)$$

In finite volume form with backward Euler time integration:

$$\rho C_p V \frac{T_i^{n+1} - T_i^n}{\Delta t} = a_W T_{i-1}^{n+1} + a_E T_{i+1}^{n+1} - a_P T_i^{n+1} + S(T_i^{n+1})V$$

This results in a linear system at each time step, which is solved using the Tri-Diagonal Matrix Algorithm (TDMA).

## Simulation Results

The simulation was executed until the maximum temperature change between successive time steps was less than $10^{-3}$ K, indicating convergence to steady-state.

- Initial center temperature: 400 K
- Final steady-state center temperature: $\approx 597.9$ K
- Time to reach steady-state: $\boxed{487.9\,\text{seconds}\ (\approx 8.13\,\text{minutes})}$

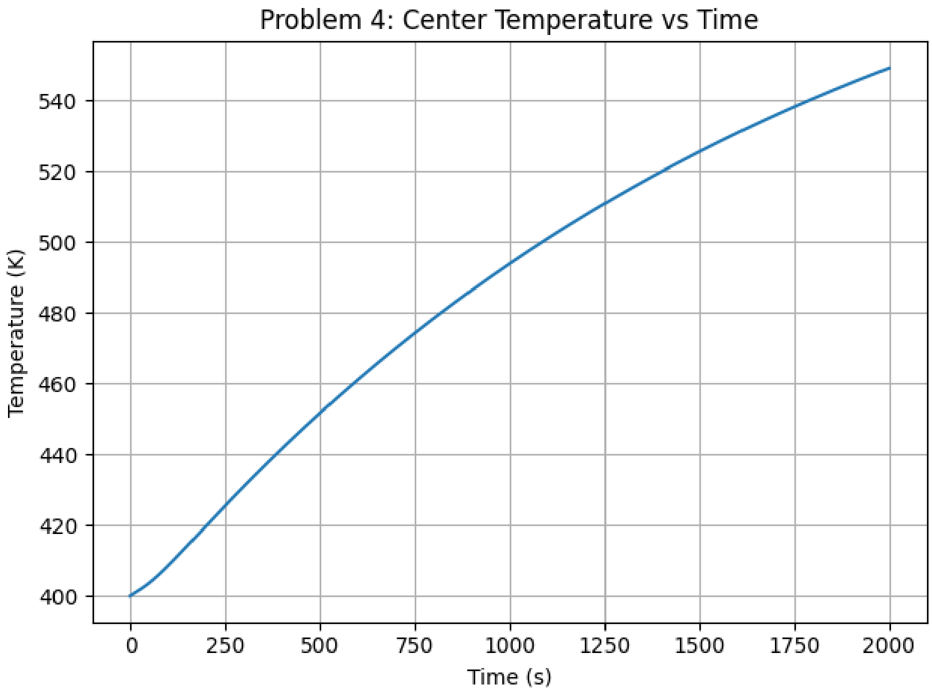


Figure 2: Center temperature vs time for transient heat conduction in the porous catalytic rod.

## Conclusion

With $N = 12$ control volumes and $\Delta t = 0.1$ s, the porous catalytic rod reaches steady-state in under 8.2 minutes. This validates the stability and efficiency of the implicit Euler method for transient thermal simulations involving nonlinear sources and temperature-dependent properties.

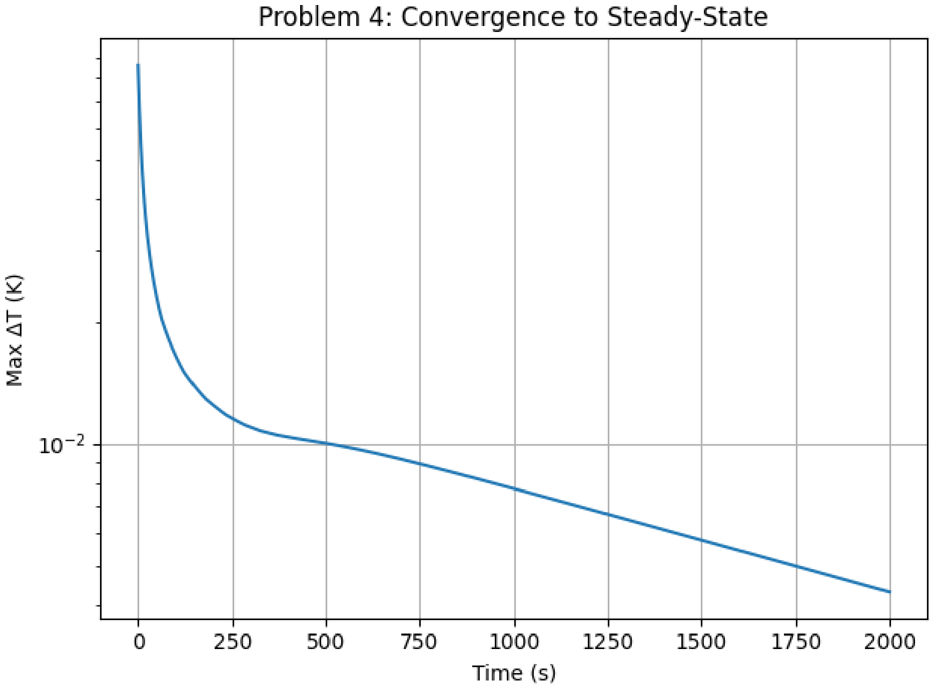


Figure 3: Convergence of the maximum temperature difference ($\Delta T$) over time.