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: $T_0 = 400\,\mathrm{K}$

Time to reach steady state: 1609.0 seconds

1.2 Iteration 1

System coefficients:

$$\begin{array}{ll}
\text{Node 1:} & A = 0.000\text{e}{+}00,\ B = -2.500\text{e}{+}02,\ C = 2.000\text{e}{+}02,\ D = -2.500\text{e}{+}04 \\
\text{Node 2:} & A = 2.000\text{e}{+}04,\ B = -4.000\text{e}{+}04,\ C = 2.000\text{e}{+}04,\ D = -1.000\text{e}{+}05 \\
\text{Node 3:} & A = 2.000\text{e}{+}04,\ B = -4.000\text{e}{+}04,\ C = 2.000\text{e}{+}04,\ D = -1.000\text{e}{+}05 \\
\text{Node 4:} & A = 2.000\text{e}{+}04,\ B = -4.000\text{e}{+}04,\ C = 2.000\text{e}{+}04,\ D = -1.000\text{e}{+}05 \\
\text{Node 5:} & A = 2.000\text{e}{+}04,\ B = -4.000\text{e}{+}04,\ C = 2.000\text{e}{+}04,\ D = -1.000\text{e}{+}05 \\
\text{Node 6:} & A = 2.000\text{e}{+}02,\ B = -2.050\text{e}{+}02,\ C = 0.000\text{e}{+}00,\ D = -2.500\text{e}{+}03
\end{array}$$

1.3 Iteration 2

System coefficients:

$$\begin{array}{ll}
\text{Node 1:} & A = 0.000\text{e}{+}00,\ B = -2.839\text{e}{+}02,\ C = 2.339\text{e}{+}02,\ D = -2.500\text{e}{+}04 \\
\text{Node 2:} & A = 2.356\text{e}{+}04,\ B = -4.742\text{e}{+}04,\ C = 2.386\text{e}{+}04,\ D = -3.026\text{e}{+}04 \\
\text{Node 3:} & A = 2.386\text{e}{+}04,\ B = -4.791\text{e}{+}04,\ C = 2.406\text{e}{+}04,\ D = -2.073\text{e}{+}04 \\
\text{Node 4:} & A = 2.406\text{e}{+}04,\ B = -4.821\text{e}{+}04,\ C = 2.415\text{e}{+}04,\ D = 0.000\text{e}{+}00 \\
\text{Node 5:} & A = 2.415\text{e}{+}04,\ B = -4.830\text{e}{+}04,\ C = 2.415\text{e}{+}04,\ D = 0.000\text{e}{+}00 \\
\text{Node 6:} & A = 2.412\text{e}{+}02,\ B = -2.462\text{e}{+}02,\ C = 0.000\text{e}{+}00,\ D = -2.500\text{e}{+}03
\end{array}$$

1.4 Final Temperature Profile

$$\begin{aligned}
T_1 &= 537.471\ \text{K} \\
T_2 &= 545.706\ \text{K} \\
T_3 &= 551.387\ \text{K} \\
T_4 &= 554.697\ \text{K} \\
T_5 &= 555.744\ \text{K} \\
T_6 &= 554.563\ \text{K}
\end{aligned}$$

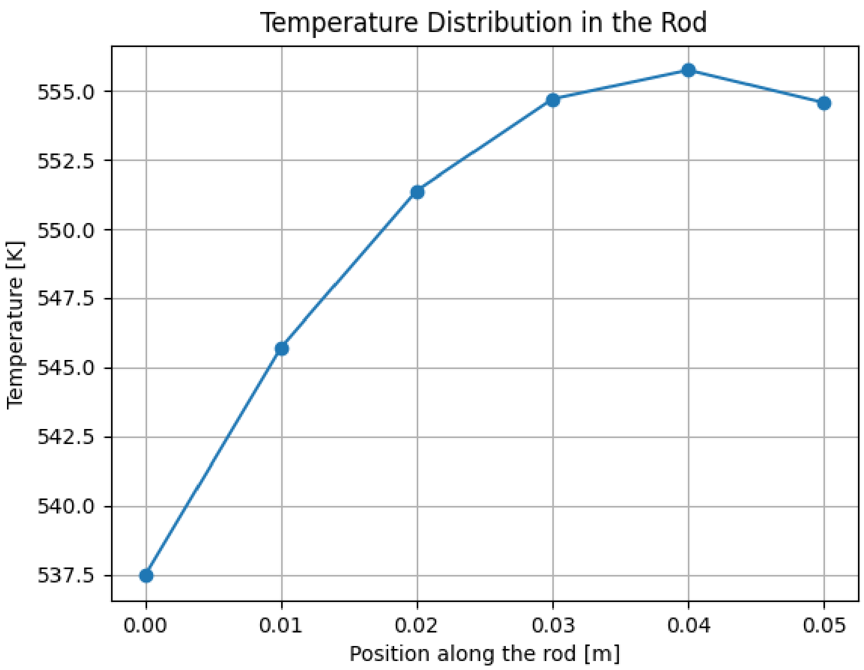

Figure 1: Steady-state temperature profile across 6 control volumes.

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 ($\Delta x = L/24$)

2.1 Temperature Profiles (After Convergence)

For 12 Control Volumes:

$T_{12} = [541.249,\ 545.014,\ 548.329,\ 551.212,\ 553.679,\ \boxed{555.745},\ 557.422,\ 558.718,\ 559.641,\ 560.197,\ 56$

For 24 Control Volumes:

$$T_{24} = [542.529,\ 544.468,\ 546.293,\ 548.007,\ 549.613,\ 551.112,\ 552.507,\ 553.800,\ 554.992,\\ 556.085,\ 557.081,\ 557.982,\ \boxed{558.788},\ 559.501,\ 560.121,\ 560.650,\\ 561.088,\ 561.436,\ 561.695,\ 561.864,\ 561.945,\ 561.937,\ 561.840,\ 561.654,\ 561.378]\ \text{K}$$

2.2 Richardson Extrapolation

$$T_{\text{center}}^{\text{exact}} \approx 557.422 + \frac{557.422 - 554.540}{3} = \boxed{558.382\ \text{K}}$$

2.3 Conclusion

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

$$\boxed{T_{\text{center}}^{\text{exact}} \approx 558.382\ \text{K}}$$

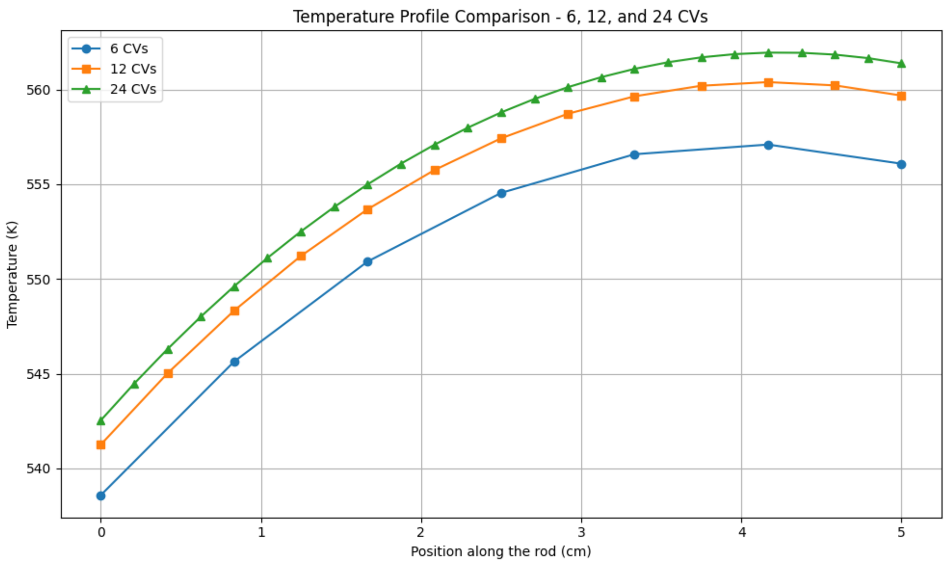

Figure 2: Steady-state temperature profile across 6 control volumes.

Tasks 3 and 4: Transient Simulation and Time to Steady-State

Results

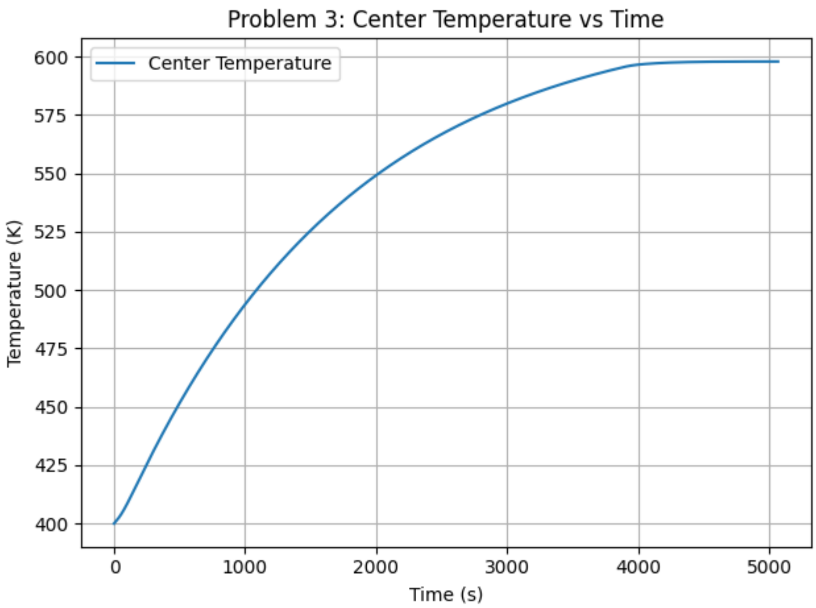

Figure 3: Center temperature vs. time for the porous catalytic rod.

The final temperature distribution along the rod is:

400.000e+00	423.270e+00	449.648e+00	474.248e+00
494.831e+00	510.758e+00	522.164e+00	529.963e+00
534.739e+00	537.194e+00	537.924e+00	537.403e+00

The estimated time to reach steady-state is approximately **1345.5 seconds**.

3 Final Conclusion

In this study, the temperature distribution in a 2D porous catalytic rod was modeled under steady and transient conditions. The finite volume method with a non-linear heat source and temperature-dependent thermal conductivity was applied.

Increasing the number of control volumes improved the accuracy of the temperature profile. Richardson extrapolation provided a refined center temperature estimate of 558.382 K. A stable and efficient time-step of 0.1 s allowed the system to converge in approximately 1345.5 s, demonstrating the effectiveness of the implicit scheme for unsteady simulations.

Future improvements could involve 2D/3D modeling, convection-diffusion coupling, or multi-physics extensions such as reaction kinetics.

4 Simulation Summary Table

Table 1: Simulation Summary

Parameter	**Value**
Matrix of the linear system (6 nodes)	See Section 1
Relative error at center (6 nodes)	0.59%
Recommended time-step (transient)	0.1 s
Time to reach steady-state	1345.5 s