Transport Homework 3

Daniel Naumov

September 22 2022

1 Problem Statement

Consider a spherical reactor with internal radius R_1=1 m and external radius R_2=1.2 m (as depicted below). An endothermic reaction takes place inside the reactor and consumes 10 W/m^3 of heat uniformly through the reactor. The thermal conductivity, k, of the reaction media (reactants and products) is $\frac{100W}{K\times m}$ while the thermal conductivity of the reactor wall is $\frac{500W}{K\times m}$. The external wall of the reactor is kept at a fixed temperature of 300 K.

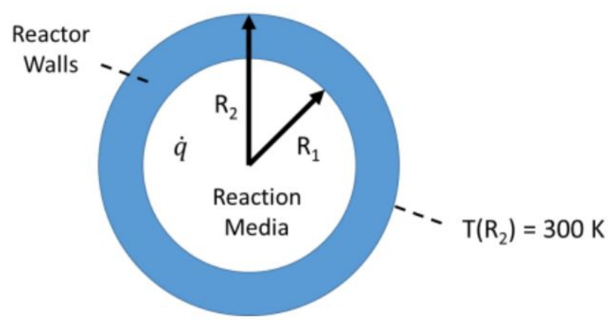

Figure 1: Spherical Reactor

The radial temperature profile across the reactor can be calculated using the heat diffusion equation:

$$k\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)\right) - \dot{q} = 0 \;\; (\dot{q} \text{ is volumetric heat consumption}) \tag{1}$$

1.1 Part I

Derive the analytical solution for the temperature profile, T(r), for the reactor described above. Your analytical solution should have two components: one for the internal region of the reactor, and one for the wall of the reactor.

Analytical Step-by-Step solution to the described reactor (inner portion):

$$k\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)\right) - \dot{q} = 0 \tag{2}$$

$$\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)\right) = \frac{\dot{q}}{k} \tag{3}$$

$$\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = \frac{\dot{q}}{k} \times r^2 \tag{4}$$

$$\left(r^2\frac{dT}{dr}\right) = \frac{\dot{q}}{3k} \times r^3 + C_1 \tag{5}$$

$$\frac{dT}{dr} = \frac{\dot{q}}{3k} \times r + \frac{C_1}{r^2} \tag{6}$$

$$T(r) = \frac{\dot{q}}{6k} \times r^2 - \frac{C_1}{r} + C_2 \tag{7}$$

Solving for C_1:

$$\left[\frac{dT}{dr}\right]_{r=0} = 0. \tag{8}$$

$$-\frac{\dot{q}}{3k} \times r = \frac{C_1}{r^2} \tag{9}$$

$$-\frac{\dot{q}}{3k} \times r^3 = C_1 \tag{10}$$

$$-\frac{\dot{q}}{3k} \times 0^3 = C_1 = 0 \tag{11}$$

Solving for C_2:

$$\left[\frac{dT}{dr}\right]_{r=r_i} = \frac{\dot{q}}{3k} \times r_i. \tag{12}$$

$$T_{r_i} = \frac{\dot{q}}{6k} \times r_i^2 - 0 + C_2 \tag{13}$$

$$T_{r_i} - \frac{\dot{q}}{6k} \times r_i^2 = C_2 \tag{14}$$

Inner T(r) equation:

$$T(r_i) = \frac{\dot{q}}{6k_M} \times r^2 + T_{r_i} - \frac{\dot{q}}{6k_M} \times r_i^2 \tag{15}$$

$$T(r_i) = \frac{\dot{q}}{6k_M} \times \left(r^2 - r_i^2\right) + T_{r_i} \tag{16}$$

Outer T(r) equation:

$$T(r_o) = T_{r_i} - \Delta T\left[\frac{1-(r_1/r)}{1-(r_1/r_2)}\right] \tag{17}$$

Combined T(r):

$$T(r) = \begin{cases} \frac{\dot{q}}{6k_M} \times (r^2 - r_i^2) + T_{r_i} & \text{if } r < r_i \\ T_{r_i} - (T_{r_i} - T_{r_o}) \left[\frac{1-(r_1/r)}{1-(r_1/r_2)}\right] & \text{if } r_i < r < r_o \end{cases} \tag{18}$$

Numerical Setup:

$$k\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)\right) - \dot{q} = 0 \tag{19}$$

$$\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)\right) = \frac{\dot{q}}{k} \tag{20}$$

$$\frac{1}{r^2} \times \left(2r\frac{dT}{dr} + r^2\frac{d^2T}{dr^2}\right) = \frac{\dot{q}}{k} \tag{21}$$

$$\frac{2}{r}\frac{dT}{dr} + \frac{d^2T}{dr^2} = \frac{\dot{q}}{k} \tag{22}$$

$$\tag{23}$$

Numerical Approximation (derivative evaluation):

$$\Delta r_j = \frac{r}{\mathrm{N}+1} \tag{24}$$

$$\left[\frac{dT}{dr}\right]_{r_j} \approx \frac{T_{j+1} - T_{j-1}}{2\Delta r} \tag{25}$$

$$\left[\frac{d^2T}{dr^2}\right]_{r_j} \approx \frac{T_{j+1} - 2T_j + T_{j-1}}{\Delta r^2} \tag{26}$$

$$\tag{27}$$

Numerical Approximation (formula and grouping)

$$\frac{T_{j+1} - 2T_j + T_{j-1}}{\Delta r^2} + \frac{2}{j\Delta r}\frac{T_{j+1} - T_{j-1}}{2\Delta r} = \frac{\dot{q}}{k} \tag{28}$$

$$\left(\frac{1}{\Delta r^2} + \frac{2}{j\Delta r^2}\right)T_{j+1} + \left(\frac{-2}{\Delta r^2}\right)T_j + \left(\frac{1}{\Delta r^2} - \frac{1}{j\Delta r^2}\right)T_{j-1} = \frac{\dot{q}}{k} \tag{29}$$

$$\left(1 + \frac{2}{j}\right)T_{j+1} + (-2)T_j + \left(1 - \frac{1}{j}\right)T_{j-1} = \frac{\dot{q}\Delta r^2}{k} \tag{30}$$

$$\tag{31}$$

$$A = 1 + \frac{1}{j} \tag{32}$$

$$B = -2 \tag{33}$$

$$C = 1 - \frac{1}{j} \tag{34}$$

I want to set up $AT_{j+1} + BT_j + CT_{j-1} = \frac{\dot{q}\Delta r^2}{k_M}$ for the points in the reactor, and $AT_{j+1} + BT_j + CT_{j-1} = 0$ for the points in the reactor walls. Applying the boundary conditions to determine what happens at j = 1, j = border, j = N. At j = 1, $AT_2 + BT_1 + CT_0 = \frac{\dot{q}\Delta r^2}{k_M}$ where CT_0 is not part of the grid. Expressing T_0 as $T(r_0) = T_b$ leads to $AT_2 + BT_1 + CT_b = \frac{\dot{q}\Delta r^2}{k_M} = AT_2 + BT_1 = \frac{\dot{q}\Delta r^2}{k_M} - CT_b$. At j = N, $300A + BT_N + CT_{N-1} = 0$. Let P be a point at the boundary between reactor and reactor wall. At j = P, $AT_{j+1} + BT_j + CT_{j-1} = \frac{\dot{q}\Delta r^2}{k_M}$.