**CM 3450**
**Fall 2008**
**Project 1**
**Due: November 21, 2008**


(Based on problem 3.8 of Adidharma and Temyandko, "Mathcad for Chemical Engineers", p. 141)

A first order reaction occur in a porous spherical catalyst pellet. Assuming negligible resistance of mass transfer outside the pellets, the mass and energy balances inside the pellet is given in terms of dimensionless radius, concentration and temperature denote by $r^*, C^*$ and $T^*$, respectively, as follows:

$$\frac{1}{r^{*2}} \frac{d}{dr^*}\left( r^{*2} \frac{dC^*}{dr^*} \right) = f(C^*, T^*)$$

$$\frac{1}{r^{*2}} \frac{d}{dr^*}\left( r^{*2} \frac{dT^*}{dr^*} \right) = -\beta\, f(C^*, T^*)$$

$$f(C^*, T^*) = \phi^2 C^* \exp\left( \gamma - \frac{\gamma}{T^*} \right)$$

Boundary Conditions:

$$\left. \frac{dC^*}{dr^*} \right|_{r^*=0} = 0 \quad \text{and} \quad C^*|_{r^*=1} = 1$$

$$\left. \frac{dT^*}{dr^*} \right|_{r^*=0} = 0 \quad \text{and} \quad T^*|_{r^*=1} = 1$$

where $\phi, \beta$ and $\gamma$ are the Thiele modulus, dimensionless heat of reaction and dimensionless activation energy, respectively.

It is known from other sources that $\beta = 0.15$ and $\gamma = 9$. However, the value of the Thiele modulus is unknown, and needs to be estimated using the set of laboratory data given in Table 1.

Table 1. Experimental Data.

| $r^*$ | $C^*$ | $T^*$ |
|---|---|---|
| 0.083 | 0.95881 | 1.00618 |
| 0.167 | 0.95943 | 1.00609 |
| 0.250 | 0.96079 | 1.00588 |
| 0.333 | 0.96278 | 1.00558 |
| 0.417 | 0.96539 | 1.00519 |
| 0.500 | 0.96859 | 1.00471 |
| 0.583 | 0.97238 | 1.00414 |
| 0.667 | 0.97675 | 1.03490 |
| 0.750 | 0.98171 | 1.00274 |
| 0.833 | 0.98725 | 1.00191 |
| 0.917 | 0.99336 | 1.00100 |
| 1.000 | 1.00000 | 1.00000 |

Try it for $\phi = 0.4, 0.5$ and 0.6, and decide which value best matches the data. Plot the concentration profile for all three cases (using curves) together with the data points (using symbols). Also plot the temperature profile for all three cases together with the data points.

Then, decided on which value of the Thiele modulus, $\phi$, is the most appropriate for catalyst pellet the yielded the data in Table 1.