06-720 Advanced Process Systems Engineering Spring, 2011

Homework 9 Due: 4/18/11

1. Consider the reactor optimization problem given by:

$$\begin{aligned} \min \quad & L - 500\int_0^L (T(t) - T_S)dt \\ s.t. \quad & \frac{dq}{dt} = 0.3(1-q(t))exp(20(1-1/T(t)),\ q(0) = 0 \\ & \frac{dT}{dt} = -1.5(T(t) - T_S) + 2/3\frac{dq}{dt},\ T(0) = 1 \end{aligned}$$

where $q(t)$ and $T(t)$ are the normalized reactor conversion and temperature, respectively, and the decision variables are $T_S \in [0.5, 1]$ and $L \in [0.5, 1.25]$.

   (a) Derive the direct sensitivity equations for the DAEs in this problem.

   (b) Using MATLAB or a similar package, apply the sequential approach to find the optimum values for the decision variables.

   (c) How would you reformulate the problem so that the path constraint $T(t) \leq 1.45$ can be enforced?

2. Consider the system of differential equations:

$$\begin{aligned} \tfrac{dz_1}{dt} &= z_2 \\ \tfrac{dz_2}{dt} &= 1600z_1 - (\pi^2 + 1600)sin(\pi t) \end{aligned}$$

   (a) Show that the analytic solution of these differential equations are the same for the initial conditions $z_1(0) = 0, z_2(0) = \pi$ and the boundary conditions $z_1(0) = z_1(1) = 0$.

   (b) Find the analytic solution for the initial and boundary value problems. Comment on the dichotomy of each system.

3. Consider the following reactor optimization problem.

$$\begin{aligned} \max \quad & c_2(1.0) \\ s.t. \quad & \frac{dc_1}{dt} = -k_1(T)c_1^2,\ c_1(0) = 1 \\ & \frac{dc_2}{dt} = k_1(T)c_1^2 - k_2(T)c_2,\ c_2(0) = 0 \end{aligned}$$

where $k_1 = 4000\ exp(-2500/T)$, $k_2 = 62000\ exp(-5000/T)$ and $T \in [298, 398]$. Discretize the temperature profile as piecewise constants over N_T periods and perform the following.

   (a) Derive the direct sensitivity equations for the DAEs in this problem.

   (b) Derive the adjoint sensitivity equations for the DAEs in this problem.

   (c) Solve using the sequential strategy with MATLAB or a similar package.

   (d) Solve using the multiple shooting strategy with MATLAB or a similar package.