ODE Practice Problems

Nonisothermal Plug-Flow Reactor

Write general MATLAB functions for integrating simultaneous nonlinear differential equations using the Euler and Runge Kutta methods. Apply these functions for the solution of differential equations that simulate a nonisotherm plug reactor, as described below:

Vapor-phase cracking of acetone, described by the following endothermic reaction:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

takes place in a jacketed tubular reactor. Pure acetone enters the reactor at a temperature of T_o=1035K and pressure of P_o=162 kPa, and the temperature of external gas in the heat exchanger is constant at T_a=1150K. Other data are as follows:

Volumetric flow rate:	$v_o=0.002 m^3/s$
Volume of the reactor:	$V_R=1 m^3$
Overall heat transfer coefficient:	$U=110\ W/m^2K$
Heat transfer area:	$a=150\ m^2/m^3$ reactor
Reaction constant:	$k=3.58 \exp[34222 *((1/1035) – (1/T))]\ s^{-1}$

Heat of reaction:

$\Delta H_R = 80770+6.8(T-298)-5.75x10^{-3}(T^2-298^2)-1.27x10^{-6}(T^3-298^3)$ J/mol

Heat capacity of acetone:	$C_{pA}=26.63 + 0.1830*T-45.86 \times 10^{-6} T^2$ J/mol.K
Heat capacity of ketene:	$C_{pB}=20.04+0.0945*T-30.95 \times 10^{-6} T^2$ J/mol.K
Heat capacity of methane:	$C_{pC}=13.39+0.077*T-18.71 \times 10^{-6} T^2$ J/mol.K

Determine the temperature profile of the gas along the length of the reactor. Assume constant pressure throughout the reactor.

Method of Solution: In order to calculate the temperature profile in the reactor, we have to solve the material balance and energy balance equations simultaneously:

Mole balance: $$\frac{dX}{dV} = \frac{-r_A}{F_{A_0}}$$

Energy balance: $$\frac{dT}{dV} = \frac{Ua(T_a-T)+r_A \Delta H_R}{F_{A_0}(C_{pA}+X*\Delta C_p)}$$

where X is the conversion of acetone, V is the volume of the reactor, $F_{A0}=C_{A0} * v_o$ is the molar flow rate of acetone at the inlet, T is the temperature of the reactor,

$\Delta C_p = C_{pB} + C_{pC} - C_{pA}$, and C_{A0} is the concentration of acetone vapor at the inlet. The reaction rate is given as

$$-r_A = kC_{A0}\frac{1-X}{1+X}\frac{T_0}{T}$$

Flow of a Non-Newtonian Fluid.

Write a general MATLAB function for solution of a boundary value problem by the shooting method. Apply this function to find the velocity profile of non-Newtonian fluid that is flowing through a circular tube as shown below (Fig. 1). Also calculate the volumetric flow rate of the fluid. The viscosity of this fluid can be described by the Carreau model:

$$\frac{\mu}{\mu_0} = [1 + (t_1\dot{\gamma})^2]^{(n-1)/2}$$

where μ is the viscosity of the fluid, μ_0 is the zero shear rate viscosity, $\dot{\gamma}$ is the shear rate, t_1 is the characteristic time, and n is a dimensionless constant.

The momentum balance for this flow, assuming the tube is very long so that end effect is negligible, results in

$$\frac{d}{dr}(r\tau_{rz}) = -\frac{\Delta P}{L}r \qquad (1)$$

Where $\Delta P/L$ is the pressure drop gradient along the pipe and the shear stress is expressed as

$$\tau_{rz} = -\mu\dot{\gamma} = -\mu\frac{dv_z(r)}{dr}$$

Therefore, Eq. (1) is a second-order ordinary differential equation, which should be solved with the following boundary conditions:

No slip at the wall: $r = R,\ v_z = 0$

Symmetry: $r = 0,\ \frac{dv_z}{dr} = 0$

The required data for the solution of this problem are:

$\mu_0 = 102.0$ Pa.s $\quad t_1 = 4.36$ s $\quad n = 0.375 \quad R = 0.1$ m $\quad -\frac{\Delta P}{L} = 20$ kPa/m

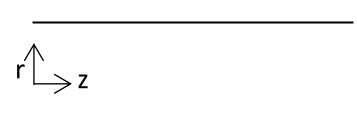

Figure 1

Method of Solution: First we define the following two variables:

Dimensionless distance: $\eta = r/R$

Dimensionless velocity: $\phi = v_z v^*$

where $v^* = (-\Delta P)R^2/L\mu_0$. Eq. (1) can be expanded and rearranged in its dimensionless form into the following second-order differential equation:

$$\frac{d^2\phi}{d\eta^2} = -\frac{\frac{1}{\eta}\frac{d\phi}{d\eta}+[1+\lambda^2(\frac{d\phi}{d\eta})^2]^{(1-n)/2}}{1-\frac{(1-n)\lambda^2(\frac{d\phi}{d\eta})}{[1+\lambda^2(\frac{d\phi}{d\eta})^2]}} \qquad (2)$$

where $\lambda = t_1 v^*/R$.

In order to obtain the canonical form of Eq. (2), we apply the following transformation:

$$y_1 = \frac{d\phi}{d\eta}$$

$$y_2 = \phi$$

The canonical form of Eq. (2) is given as

$$\frac{dy_1}{d\eta} = -\frac{\frac{1}{\eta}y_1+[1+\lambda^2 {y_1}^2]^{(1-n)/2}}{1-\frac{(1-n)\lambda^2 y_1}{[1+\lambda^2 {y_1}^2]}} \qquad (3)$$

$$\frac{dy_2}{d\eta} = y_1 \qquad (4)$$

The set of nonlinear ordinary differential equations (3) and (4) should be solved with the following boundary conditions:

$$y_1(0) = y_{1,0} = 0 \qquad (5)$$

$$y_2(1) = y_{2,f} = 0 \qquad (6)$$

The initial value $y_1(0)$ is known, but the initial value $y_2(0)$ must be guessed. We designate this guess, in accordance with Eq. (5.120), as follows:

$$y_2(0) = \gamma = \frac{\left[\frac{(-\Delta P)R^2}{4L\mu_0}\right]}{v^*} = \frac{1}{4} \qquad (7)$$

The right-hand side of Eq. (7) corresponds to the velocity of the fluid at the center of the pipe if it was a Newtonian fluid with the viscosity μ_0.

The complete set of equations for the solution of this two-point boundary-value problem consists of:

1. The four system equations with their known boundary values [Eqs. (3)-(6)]

2. The guessed initial condition for y_2 [Eq. (7)]
3. Construction of the Jacobian matrix
4. Calculation of the δy vector
5. Correcting the guessed initial conditions.

Once the velocity profile is determined, the flow rate of the fluid can be calculated from the following integral formula:

$$Q = \int_0^R 2\pi r v_z dr$$