PROBLEMS

Problem 4-1

The equation describing the change in the level (H) of a tank is given by:

$$\frac{dH}{dt} = \frac{1}{141}(45 - 12H^{4/7})$$

$$H = 2 \text{ at } t = 0$$

(a) Determine the level in the tank after 20 minutes using explicit Euler, Runge-Kutta order 2 & 4 and implicit Euler methods. Choose a step size of 5 minute.

Problem 4-2:

A heating tank contains 5000lb of oil which is initially at 60°F. Saturated steam at 300°F is transferring heat to oil in the tank through coil at a rate which is expressed by the equation:

$$Q = h(T_s - T)$$

where T is the uniform temperature of the oil, T_s is saturated steam temperature, and h is the heat transfer coefficient. Assuming that the mass flow rates of the feed and the discharge from the tank are constant, the energy balance equation for this tank has the form

$$V\rho Cp\frac{dT}{dt} = mCp(T_i - T) + Q$$

where V is the volume of the tank, ρ is the oil density and Cp is the heat capacity of the oil .

For the given data:

$V\rho$ = 5000 lb, Cp = 0.5Btu/lb F, m = 1000 lb/h, T_i = 60 °F, T_s = 300°F, h = 300 Btu/h°F

Calculate analytically and numerically the time in minutes to raise the oil temperature from 60^oF to 90^oF

Problem 4-3:

The production of methyl bromide is an irreversible elementary liquid-phase reaction

$$CH_3NH_2 + CNBr \rightarrow NCNH_2 + CH_3Br; \qquad (A + B \rightarrow C + D)$$

that is carried out in a semibatch reactor. An aqueous solution of *B* at a concentration of 0.025 mol/cm^3 is to be fed at a rate of 0.05 cm^3/s to an aqueous solution of bromine cyanide (A) contained in a glass-lined reactor. The initial volume of fluid in the tank is 5 cm^3 with bromine cyanide concentration of 0.05 mol/cm^3. The specific reaction rate constant is k = 2.2 cm^3 /s mol.

- Show that the model equation can be written as:

$$\frac{dX}{dt} = \frac{k(1-X)(F_{Bo}t - N_{Ao}X)}{V_o + v_o t}$$

where *X* is the conversion of *A*.

- Solve for the conversion of bromine cyanide and the concentration of methyl bromide.

Problem 4-4:

The dynamics of a gravity-flow tank can be expressed by the following ODE's where *H*(ft) is the height of the tank and *V*(ft/s) is the velocity of the liquid:

$$\frac{dH}{dt} = 0.211 - 0.824V$$

$$\frac{dV}{dt} = 0.0107H - 0.00405V^2$$

(a) Determine the steady state values of the height and velocity.

(b) Using explicit Euler's method with a step size of 5 seconds determine the height and velocity of the tank after 20 seconds when the initial conditions are $H = 2.5$ ft and $V = 3.6$ ft/s.

(c) Solve the same problem using a second order Runge-Kutta method.

Problem 4-5:

The equation for the steady state heat conduction through a large flat slab with a temperature- dependent heat conductivity ($\lambda = \lambda_0 + \alpha T$) is given below. The solution describes the temperature $T(x)$ as a function of x through the slab.

$$\frac{d}{dx}\left((\lambda_o + \alpha T)\frac{dT}{dx}\right) = 0$$

$$T(0) = 5, \qquad \frac{dT}{dx}|_{x=0} = 1$$

(a) Replace the given equation by two (or more) first order differential equations by introducing new variables .

(b) Solve the differential equations using explicit Euler method

Problem 4-6:

Consider the following autocatalytic reaction in a CSTR:

$$A + 2B \rightarrow 3B; \;\; B \rightarrow C$$

The mathematical model is the following:

$$\frac{dx}{dt} = \frac{1-x}{\theta} - xy^2$$

$$\frac{dy}{dt} = \frac{\beta - y}{\theta} - xy^2 + \kappa y$$

where x, y are dimensionless concentrations of the reactant A and the autocatalyst B. For the following system parameters:

$$\theta = 10,\ \beta = 0.1,\ \kappa = 0.1$$

(a) Solve the given system for the steady state case.

(b) Simulate the transient behavior of the system starting from initial conditions: $x_0 = 0.01$, $y_0 = 0.1$

Problem 4-7

A mathematical model for a non-isothermal, continuous, stirred tank reactor in which two, exothermic, first order, irreversible reactions $A \rightarrow C, B \rightarrow C$ are occurring in parallel is given by:

$$\frac{dx_1}{dt} = 1 - x_1 - x_1 Da_1 e^{\gamma_1 T/(1+T)}$$

$$\frac{dx_2}{dt} = 1 - x_2 - x_2 Da_2 e^{\gamma_2 T/(1+T)}$$

$$\frac{dT}{dt} = \alpha\left(\beta_1 x_1 Da_1 e^{\gamma_1 T/(1+T)} + \beta_2 x_2 Da_2 e^{\gamma_2 T/(1+T)} - T\right)$$

where x_1, x_2 are dimensionless concentrations of the reactants (A,B) and T is the reactor temperature. For the system parameters: $Da_1 = Da_2 = 2.75$, $\beta_1 = \beta_2 = 0.04$, $\gamma_1 = \gamma_2 = 25$ and $\alpha = 250$, find the steady state values for this model using an ODEs solver starting with zero initial conditions .

Problem 4.8

The following model was proposed for a one-dimensional tubular reactor with constant wall temperature, a single reaction, and a fluid of constant density:

$$u\frac{dp}{dz} = -\frac{MP\rho_b}{\rho_g}$$

$$u\frac{dT}{dz} = -\frac{\Delta H\rho_b}{Cp}r - \frac{2U}{RCp}(T - T_M)$$

$$r = pP_B^o e^{(-\frac{a}{T}+b)}$$

At $z = 0$, $p = p^o$, $T = T_M$ (z = length along reactor). For the napthalene oxidation reaction, the following values of the parameters apply:

ρ_g		= 1.293 kg/m^3
M	(molecular wieght)	= 29.28 kg/kmol
p_o	(inlet partial pressure, atm)	
ρ_b	(bulk density)	= 1300 kg/m^3
$-\Delta H$	(heat of reaction)	= 307000 kcal /kmol
p	(partial pressure of naphthalene, atm)	
P		= 1 atm.
Cp	(heat capacity)	= 0.323 kcal/(m^3 ^{o}C)
U	(overall heat transfer coefficient)	= 82.7 kcal/m^2 h ^{o}C
p_B^o		= 0.208 kmol/atm kg
a		= 13636 K
b		= 19.837
u	linear velocity	= 3600 m/hr
R	radius	= 0.0125 m
T_M	wall temperature	= 625 K

(a)For an inlet and wall temperature of 625 ^{o}K and total pressure of 1 atm, compute the partial pressure and temperature profiles along the reactor length for a distance of 1 m for naphthalene inlet partial pressure of 0.011, 0.013, 0.015,0.017, 0.018, 0.019 atm.

(b) Repeat same problem for adiabatic operation.

Problem 4.9

For a semi-batch reactor, the unsteady state mass balance for the reactant A with second order kinetics is given by:

$$\frac{dn_A}{dt} Q_0 C_{A0} - \frac{k n_A^2}{Q_0 t + V_0}$$

where $n_A = 0$ at $t = 0$. The parameters for this problem are $C_A = 1.0$ mol/liter, $k = 0.14$liter/mol.sec, $Q_0 = 10.0$liter/sec, $V_0 = 50$ liters. Taking the step size of 5 sec calculate n_A using 4th order Runge-Kutta and explicit Euler methods up to $t = 50$ sec.

Problem 4.10

Find the time necessary to fill a tank of cross sectional area 1.5 m^2 to its steady state liquid height of 4 m when the tank is having a valve at the bottom with a valve coefficient, (c), equal to 10 m^3/min $m^{0.5}$, and the tank is being fed with a constant feed flow rate of 20 m^3/min. The dynamic equation for the level is given by:

$$A\frac{dh}{dt} = F - ch^{0.5}, \qquad h(0) = 0$$

Problem 4.11

A mathematical model for the isolated population dynamics of a typical autoregenerative biological system is given by

$$\frac{dx}{dt} = \alpha x(\mu - x), \qquad x(0) = 0$$

where

x is the instantaneous population variable

α is a characteristic constant of the biological system = 0.5

μ is the independent 'source' variable = 0.2

Solve for the values of x until time 20.

Problem 4.12

The dynamic behavior of the liquid level in a certain cylindrical storage tank is modeled by:

$$A\frac{dh}{dt} = F_i - ch^{3/2}$$

where A is the uniform cross-sectional area (m^2); F_i is the inlet flow rate (m^3/min); h is the liquid level (m) ; and c is a constant. This tank with c = 0.5 m$^{7/3}$/min, A = 0.25 m^2, and whose total height is 1 m, had a steady state liquid level of 0.512 m when operating at initial steady state flow rate of 0.32 m^3/min. It is believed that if the flow rate were to increase suddenly from this initial value to a new value of 0.52 m^3/min, and remains there will in fact cause the tank to overflow .

(a) Confirm or refute this statement.

(b) If the tank will overflow, determine the time in minute at which the tank will overflow.

Problem 4.13

A mathematical model for the level of gasoline in a hemispherical storage tank is given by

$$\frac{dL}{dt} = \frac{1}{\pi}\frac{1}{(2RL - L^2)}(F_i - cL^{0.5})$$

Given a specific tank with parameters R = 2m, and c = 1.5 (m$^{5/2}$/min), operating at initial steady state conditions : F_i = 1.35 m^3/min, $h(0)$ = 0.81 m, obtain the response of the gasoline to a step change in F_i from the initial value to 1.8 m^3/min .

Problem 4.14

The dynamic behavior of the isothermal series/parallel Van de Vusse reaction taking place in a CSTR may be modeled by the following equations:

$$\frac{dx_1}{dt} = -50x_1 - 10x_1^2 + (10 - x_1)\mu$$

$$\frac{dx_2}{dt} = 50x_1 - 100x_2 - x_2\mu$$

where x_1, x_2, are, respectively the dimensionless reactant and product concentration in the reactor and μ is the dimensionless dilution rate .

(a) Given an operating steady state value of μ = 17.5, obtain from the modeling equations the corresponding steady state values for x_1 and x_2.

(b) Obtain a simulation of the process response to a step change in the dilution rate from 17.5 to 30.0 .

Problem 4.15

A reactor used for the free-radical polymerization of methyl methacrylate is modeled by

$$\frac{dx_1}{dt} = 3(6 - x_1) - 1.4x_1x_2^{0.5}$$

$$\frac{dx_2}{dt} = 50u - 3x_2$$

$$\frac{dx_3}{dt} = -0.001x_1x_2^{0.5} + 0.035x_2 - 10x_4$$

$$\frac{dx_4}{dt} = 130x_1x_2^{0.5} - 10x_4$$

x_1, x_2, x_3 and x_4 represent the dimensionless monomer concentration, initiator concentration, bulk zeroth moment, and bulk first moment; and u is the volumetric flow rate of the initiator .

(a) Given an operating steady-state value $u = 0.02$ obtain from the modeling equations the corresponding steady state values .

(b) Starting from these steady state conditions, obtain the response of the system to a 25% increase in u .

Problem 4.16

An exothermic reaction, $A \rightarrow B$, takes place adiabatically in a stirred tank reactor. The liquid reaction occurs at constant volume in a 1000 gal reactor. The reaction can be considered to be first order and irreversible with rate constant given by:

$$k = 2.4 \times 10^{15} e^{-20000/T} \text{ (min}^{-1}\text{)}$$

where T is in R.

The mathematical model consists of the following material and energy balance equations :

$$V\frac{dC_A}{dt} = q(C_{Ai} - C_A) - VkC_A$$

$$V\rho Cp\frac{dT}{dt} = wCp(T_i - T) + (-\Delta H)VkC_A$$

The nominal steady state conditions are

$T_{ss} = 150^{o}$F, $C_{Ai,ss} = 0.8$ mol/ft^3 $q = 20$gal/min

and the physical property data for the mixture are:

$Cp = 0.8$ Btu/lb^{o}F, $\rho = 52$ lb/ft^3, $\Delta H = 500$ kJ/mol

(a) Find the steady state values of the reactant concentration $c_{A,ss}$ and reactor temperature T_{ss}

(b) For a 20% increase in the feed temperature, obtain a simulation of the system response.

Problem 4.17

A heating tank contains 5000lb of oil which is initially at 60^{o}F. Saturated steam at 300^{o}F is transferring heat to oil in the tank through coil at a rate which is expressed by the equation:

$$Q = h(T_s - T)$$

where T is the uniform temperature of the oil, T_s is saturated steam temperature, and h is the heat transfer coefficient. Assuming that the mass flow rates of the feed and the discharge from the tank are constant, the energy balance equation for this tank has the form

$$V\rho Cp\frac{dT}{dt} = mCp(T_i - T) + Q$$

where V is the volume of the tank, ρ is the oil density, Cp is the heat capacity of the oil .

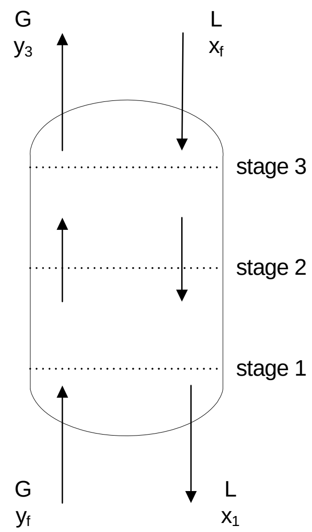
For the given data:

$V\rho = 5000$ lb, $Cp = 0.5$Btu/lb F, $m = 1000$ lb/h, $T_i = 60$ ^{o}F, $T_s = 300^{o}$F, $h = 300$ Btu/h^{o}F

Calculate analytically and numerically the time in minutes to raise the oil temperature from 60°F to 90°F

Problem 4.18

The following model was obtained for a three stage absorber shown in Figure below. Assuming constant liquid holdup *H*, perfect mixing on each stage, and neglecting the holdup of gas the component material balance for any stage *i* is



$$H\frac{dx_i}{dt} = G(y_{i-1} - y_i) + L(x_{i+1} - x_i)$$

where y_i and x_i denotes gas and liquid of the absorbed component . Assume also the molar liquid and gas flow rates, i.e., *L* and *G* are constants .

System data:

$x_f = 0.01$, $y_f = 0.06$, $L = 40.8$ lb/min, $G = 66.7$ lb/min

(a) Assuming a linear equilibrium relation:

$$y_i = 0.72\, x_i$$

For the given system parameters, find the steady state values for all x_i then obtain the response of the system for a 10% increase in gas phase concentration of the absorbed component (y_f):

(b) Repeat part (a) for the nonlinear equilibrium relation:

$$y_i = 0.05 + 0.7x_i + 0.1x_i^2$$

Problem 4.19:

The design equation for the isothermal catalytic cracking of a gas oil $A \rightarrow$Products in a moving bed reactor is given by

$$F_{Ao}\frac{dX}{dW} = a - r_A$$

where F_{A0} is the molar flow rate of A to the reactor, X is the conversion and W is the mass of the catalyst. The catalyst activity a is changing according to the deactivation equation:

$$\frac{da}{dW} = -0.072a$$

Determine the conversion that can be achieved in the reactor using the following data: The reactor contains 22 kg of catalyst, the gas oil is fed at a rate of 30 mol/min at a concentration of 0.075 mol/cm^3 and the reaction follows the rate :

$$r_A = 0.6\, C_A^2 = 0.6\, C_{A0}^2\, (1 - X)$$