THE USE OF MATHEMATICAL SOFTWARE PACKAGES IN CHEMICAL ENGINEERING

A COLLECTION OF REPRESENTATIVE PROBLEMS IN CHEMICAL ENGINEERING FOR SOLUTION BY NUMERICAL METHODS

Mathematical Software - Session 12*

Michael B. Cutlip, Department of Chemical Engineering, Box U-222, University of Connecticut, Storrs, CT 06269-3222 (mcutlip@uconnvm.uconn.edu)

John J. Hwalek, Department of Chemical Engineering, University of Maine, Orono, ME 04469 (hwalek@maine.maine.edu)

H. Eric Nuttall, Department of Chemical and Nuclear Engineering, University of New Mexico, Albuquerque, NM 87134-1341 (nuttall@unm.edu)

Mordechai Shacham, Department of Chemical Engineering, Ben-Gurion University of the Negev, Beer Sheva, Israel 84105 (shacham@bgumail.bgu.ac.il)

Additional Contributors:

Joseph Brule, John Widmann, Tae Han, and Bruce Finlayson, Department of Chemical Engineering, University of Washington, Seattle, WA 98195-1750 (finlayson@cheme.washington.edu)

Edward M. Rosen, EMR Technology Group, 13022 Musket Ct., St. Louis, MO 63146 (EMRose@compuserve.com)

Ross Taylor, Department of Chemical Engineering, Clarkson University, Potsdam, NY 13699-5705 (taylor@sun.soe.clarkson.edu)

INTRODUCTION

This collection of problems was developed for Session 12 at the ASEE Chemical Engineering Summer School held in Snowbird, Utah on August 13, 1997. These problems are intended to utilize the basic numerical methods in problems which are appropriate to a variety of chemical engineering subject areas. The problems are titled according to the chemical engineering principles which are used, the problems are arranged according to the numerical methods which are applied as summarized in Table 1.

The problem has been solved by each of the mathematical packages: Excel, Maple, Mathcad*, MATLAB, Mathematica*, and Polymath*. The CACHE Corporation has made available this problem set as well as the individual package writeups

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and problem solutions at http://www.che.utexas.edu/cache/. The materials are also available via anonymous FTP from ftp.engr.uconn.edu in directory /pub/ASEE. The problem set and details of the various solutions are given in separate documents as Adobe PDF files. Additionally, the problem sets are available for the various mathematical package as working files which can be downloaded for execution with the mathematical software. This method of presentation should indicate the convenience and strengths/weaknesses of each of the mathematical software packages and provides working solutions.

The selection of problems has been coordinated by M. B. Cutlip who served as the session chairman. The particular co-author who has considerable experience with a particular mathematical package is responsible for the solution with that package*.

Excel** - Edward M. Rosen, EMR Technology Group

Maple** - Ross Taylor, Clarkson University

Mathematica** - H. Eric Nuttall, University of New Mexico

Mathcad** - John J. Hwalek, University of Maine

MATLAB** - Joseph Brule, John Widmann, Tae Han, and Bruce Finlayson, Department of Chemical Engineering, University of Washington

POLYMATH** - Michael B. Cutlip, University of Connecticut and Mordechai Shacham, Ben-Gurion University of the Negev

This selection of problems should help chemical engineering faculty evaluate which mathematical problem solving package they wish to use in their courses and should provide some typical problems in various courses which can be utilized.

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Table 1 Selection of Problems Solutions Illustrating Mathematical Software

COURSE	PROBLEM TITLE	MATHEMATICAL MODEL	PROBLEM
Introduction to Ch. E.	Molar Volume and Compressibility Factor from Van Der Waals Equation	Single Nonlinear Equation	1
Introduction to Ch. E.	Steady State Material Balances on a Separation Train*	Simultaneous Linear Equations	2
Mathematical Methods	Vapor Pressure Data Representation by Polynomials and Equations	Polynomial Fitting, Linear and Nonlinear Regression	3
Thermodynamics	Reaction Equilibrium for Multiple Gas Phase Reactions*	Simultaneous Nonlinear Equations	4
Fluid Dynamics	Terminal Velocity of Falling Particles	Single Nonlinear Equation	5
Heat Transfer	Unsteady State Heat Exchange in a Series of Agitated Tanks*	Simultaneous ODE's with known initial conditions.	6
Mass Transfer	Diffusion with Chemical Reaction in a One Dimensional Slab	Simultaneous ODE's with split boundary conditions.	7
Separation Processes	Binary Batch Distillation**	Simultaneous Differential and Nonlinear Algebraic Equations	8
Reaction Engineering	Reversible, Exothermic, Gas Phase Reaction in a Catalytic Reactor*	Simultaneous ODE's and Algebraic Equations	9
Process Dynamics and Control	Dynamics of a Heated Tank with PI Temperature Control**	Simultaneous Stiff ODE's	10

* Problem originally suggested by H. S. Fogler of the University of Michigan
** Problem preparation assistance by N. Brauner of Tel-Aviv University

These problem are taken in part from a new book entitled "Problem Solving in Chemical Engineering with Numerical Methods" by Michael B. Cutlip and Mordechai Shacham to be published by Prentice-Hall in 1999.

1. MOLAR VOLUME AND COMPRESSIBILITY FACTOR FROM VAN DER WAALS EQUATION

1.1 Numerical Methods

Solution of a single nonlinear algebraic equation.

1.2 Concepts Utilized

Use of the van der Waals equation of state to calculate molar volume and compressibility factor for a gas.

1.3 Course Useage

Introduction to Chemical Engineering, Thermodynamics.

1.4 Problem Statement

The ideal gas law can represent the pressure-volume-temperature (PVT) relationship of gases only at low (near atmospheric) pressures. For higher pressures more complex equations of state should be used. The calculation of the molar volume and the compressibility factor using complex equations of state typically requires a numerical solution when the pressure and temperature are specified.

The van der Waals equation of state is given by

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT \tag{1}$$

where

$$a = \frac{27}{64}\left(\frac{R^2 T_c^2}{P_c}\right) \tag{2}$$

and

$$b = \frac{R T_c}{8 P_c} \tag{3}$$

The variables are defined by

P = pressure in atm

V = molar volume in liters/g-mol

T = temperature in K

R = gas constant (R = 0.08206 atm·liter/g-mol·K)

T_c = critical temperature (405.5 K for ammonia)

P_c = critical pressure (111.3 atm for ammonia)

Reduced pressure is defined as

$$P_r = \frac{P}{P_c} \tag{4}$$

and the compressibility factor is given by

$$Z = \frac{PV}{RT} \tag{5}$$

(a) Calculate the molar volume and compressibility factor for gaseous ammonia at a pressure P = 56 atm and a temperature T = 450 K using the van der Waals equation of state.
(b) Repeat the calculations for the following reduced pressures: P_r = 1, 2, 4, 10, and 20.
(c) How does the compressibility factor vary as a function of P_r?

2. STEADY STATE MATERIAL BALANCES ON A SEPARATION TRAIN

2.1 Numerical Methods

Solution of simultaneous linear equations.

2.2 Concepts Utilized

Material balances on a steady state process with no recycle.

2.3 Course Useage

Introduction to Chemical Engineering.

2.4 Problem Statement

Xylene, styrene, toluene and benzene are to be separated with the array of distillation columns that is shown below where F, D, B, D1, B1, D2 and B2 are the molar flow rates in mol/min.

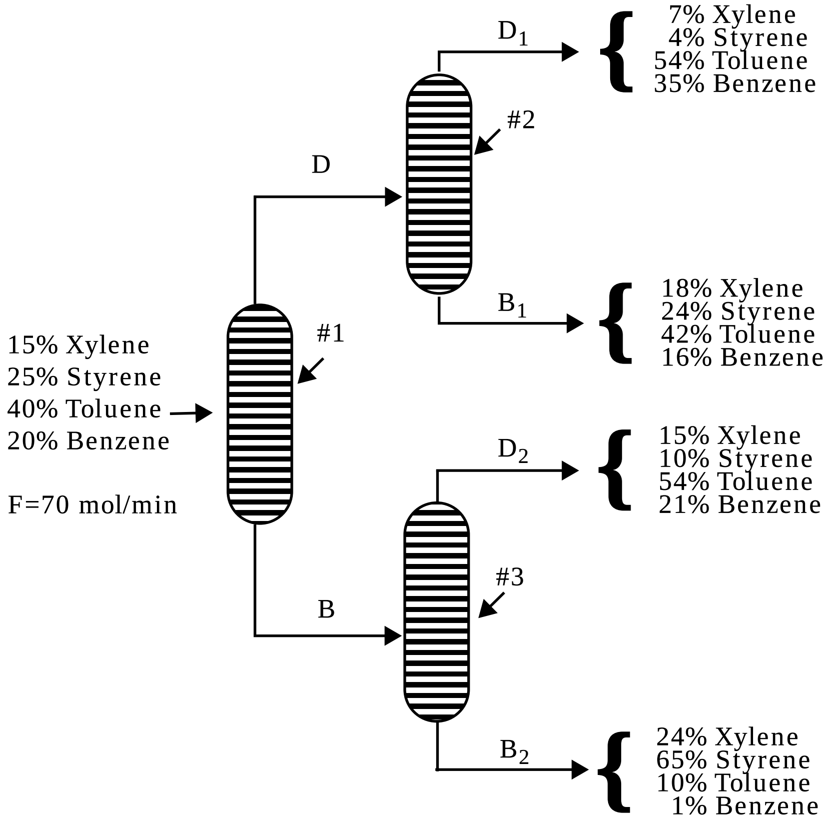

Figure 1 Separation Train

Material balances on individual components on the overall separation train yield the equation set

$$\begin{aligned}
\text{Xylene: } & 0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15 \times 70 \\
\text{Styrene: } & 0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 0.25 \times 70 \\
\text{Toluene: } & 0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 0.40 \times 70 \\
\text{Benzene: } & 0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.20 \times 70
\end{aligned} \tag{6}$$

Overall balances and individual component balances on column #2 can be used to determine the molar flow rate and mole fractions from the equation of stream D from

$$\begin{aligned}
& \text{Molar Flow Rates: } D = D_1 + B_1 \\
\text{Xylene: } & X_{Dx}D = 0.07D_1 + 0.18B_1 \\
\text{Styrene: } & X_{Ds}D = 0.04D_1 + 0.24B_1 \\
\text{Toluene: } & X_{Dt}D = 0.54D_1 + 0.42B_1 \\
\text{Benzene: } & X_{Db}D = 0.35D_1 + 0.16B_1
\end{aligned} \tag{7}$$

where X_{Dx} = mole fraction of Xylene, X_{Ds} = mole fraction of Styrene, X_{Dt} = mole fraction of Toluene, and X_{Db} = mole fraction of Benzene.

Similarly, overall balances and individual component balances on column #3 can be used to determine the molar flow rate and mole fractions of stream B from the equation set

$$\begin{aligned}
& \text{Molar Flow Rates: } B = D_2 + B_2 \\
\text{Xylene: } & X_{Bx}B = 0.15D_2 + 0.24B_2 \\
\text{Styrene: } & X_{Bs}B = 0.10D_2 + 0.65B_2 \\
\text{Toluene: } & X_{Bt}B = 0.54D_2 + 0.10B_2 \\
\text{Benzene: } & X_{Bb}B = 0.21D_2 + 0.01B_2
\end{aligned} \tag{8}$$

(a) Calculate the molar flow rates of streams D_1, D_2, B_1 and B_2.
(b) Determine the molar flow rates and compositions of streams *B* and *D*.

3. Vapor Pressure Data Representation by Polynomials and Equations

3.1 Numerical Methods

Regression of polynomials of various degrees. Linear regression of mathematical models with variable transformations. Nonlinear regression.

3.2 Concepts Utilized

Use of polynomials, a modified Clausius-Clapeyron equation, and the Antoine equation to model vapor pressure versus temperature data

3.3 Course Useage

Mathematical Methods, Thermodynamics.

3.4 Problem Statement

Table (2) presents data of vapor pressure versus temperature for benzene. Some design calculations

Table 2 Vapor Pressure of Benzene (Perry[3])

Temperature, *T* (°C)	**Pressure, *P* (mm Hg)**
-36.7	1
-19.6	5
-11.5	10
-2.6	20
+7.6	40
15.4	60
26.1	100
42.2	200
60.6	400
80.1	760

require these data to be accurately correlated by various algebraic expressions which provide P in mmHg as a function of T in °C.

A simple polynomial is often used as an empirical modeling equation. This can be written in general form for this problem as

$$P = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + \ldots + a_n T^n \quad \textbf{(9)}$$

where $a_0 \ldots a_n$ are the parameters (coefficients) to be determined by regression and n is the degree of the polynomial. Typically the degree of the polynomial is selected which gives the best data representation when using a least-squares objective function.

The Clausius-Clapeyron equation which is useful for the correlation of vapor pressure data is given by

$$\log(P) = A - \frac{B}{T + 273.15} \quad \textbf{(10)}$$

where P is the vapor pressure in mmHg and T is the temperature in °C. Note that the denominator is just the absolute temperature in K. Both A and B are the parameters of the equation which are typically determined by regression.

The Antoine equation which is widely used for the representation of vapor pressure data is given by

$$\log(P) = A - \frac{B}{T + C} \quad \textbf{(11)}$$

where typically P is the vapor pressure in mmHg and T is the temperature in °C. Note that this equation has parameters A, B, and C which must be determined by nonlinear regression as it is not possible to linearize this equation. The Antoine equation is equivalent to the Clausius-Clapeyron equation when C = 273.15.

(a) Regress the data with polynomials having the form of Equation (9). Determine the degree of polynomial which best represents the data.
(b) Regress the data using linear regression on Equation (10), the Clausius-Clapeyron equation.
(c) Regress the data using nonlinear regression on Equation (11), the Antoine equation.

4. Reaction Equilibrium for Multiple Gas Phase Reactions

4.1 Numerical Methods

Solution of systems of nonlinear algebraic equations.

4.2 Concepts Utilized

Complex chemical equilibrium calculations involving multiple reactions.

4.3 Course Useage

Thermodynamics or Reaction Engineering.

4.4 Problem Statement

The following reactions are taking place in a constant volume, gas-phase batch reactor.

$$A + B \leftrightarrow C + D$$
$$B + C \leftrightarrow X + Y$$
$$A + X \leftrightarrow Z$$

A system of algebraic equations describes the equilibrium of the above reactions. The nonlinear equilibrium relationships utilize the thermodynamic equilibrium expressions, and the linear relationships have been obtained from the stoichiometry of the reactions.

$$\begin{aligned} &K_{C1} = \frac{C_C C_D}{C_A C_B} \qquad K_{C2} = \frac{C_X C_Y}{C_B C_C} \qquad K_{C3} = \frac{C_Z}{C_A C_X} \\ &C_A = C_{A0} - C_D - C_Z \qquad C_B = C_{B0} - C_D - C_Y \\ &C_C = C_D - C_Y \qquad C_Y = C_X + C_Z \end{aligned} \tag{12}$$

In this equation set C_A, C_B, C_C, C_D, C_X, C_Y and C_Z are concentrations of the various species at equilibrium resulting from initial concentrations of only C_{A0} and C_{B0}. The equilibrium constants K_{C1}, K_{C2} and K_{C3} have known values.

Solve this system of equations when $C_{A0} = C_{B0} = 1.5$, $K_{C1} = 1.06$, $K_{C2} = 2.63$ and $K_{C3} = 5$ starting from four sets of initial estimates.

(a) $C_D = C_X = C_Z = 0$

(b) $C_D = C_X = C_Z = 1$

(c) $C_D = C_X = C_Z = 10$

5. TERMINAL VELOCITY OF FALLING PARTICLES

5.1 Numerical Methods

Solution of a single nonlinear algebraic equation..

5.2 Concepts Utilized

Calculation of terminal velocity of solid particles falling in fluids under the force of gravity.

5.3 Course Useage

Fluid dynamics.

5.4 Problem Statement

A simple force balance on a spherical particle reaching terminal velocity in a fluid is given by

$$v_t = \sqrt{\frac{4g(\rho_p - \rho)D_p}{3C_D\rho}} \qquad \textbf{(13)}$$

where v_t is the terminal velocity in m/s, g is the acceleration of gravity given by g = 9.80665 m/s^2, ρ_p is the particles density in kg/m^3, ρ is the fluid density in kg/m^3, D_p is the diameter of the spherical particle in m and C_D is a dimensionless drag coefficient.

The drag coefficient on a spherical particle at terminal velocity varies with the Reynolds number (Re) as follows (pp. 5-63, 5-64 in Perry[3]).

$$C_D = \frac{24}{Re} \qquad \text{for} \qquad Re < 0.1 \qquad \textbf{(14)}$$

$$C_D = \frac{24}{Re}(1 + 0.14Re^{0.7}) \qquad \text{for} \qquad 0.1 \le Re \le 1000 \qquad \textbf{(15)}$$

$$C_D = 0.44 \qquad \text{for} \qquad 1000 < Re \le 350000 \qquad \textbf{(16)}$$

$$C_D = 0.19 - 8\times10^4 / Re \qquad \text{for} \qquad 350000 < Re \qquad \textbf{(17)}$$

where $Re = D_p v_t \rho / \mu$ and μ is the viscosity in Pa·s or kg/m·s.

(a) Calculate the terminal velocity for particles of coal with ρ_p = 1800 kg/m^3 and D_p = 0.208×10^{-3} m falling in water at T = 298.15 K where ρ = 994.6 kg/m^3 and $\mu = 8.931\times10^{-4}$ kg/m·s.

(b) Estimate the terminal velocity of the coal particles in water within a centrifugal separator where the acceleration is 30.0 g.

6. HEAT EXCHANGE IN A SERIES OF TANKS

6.1 Numerical Methods

Solution of simultaneous first order ordinary differential equations.

6.2 Concepts Utilized

Unsteady state energy balances, dynamic response of well mixed heated tanks in series.

6.3 Course Useage

Heat Transfer.

6.4 Problem Statement

Three tanks in series are used to preheat a multicomponent oil solution before it is fed to a distillation column for separation as shown in Figure (2). Each tank is initially filled with 1000 kg of oil at 20°*C*. Saturated steam at a temperature of 250°*C* condenses within coils immersed in each tank. The oil is fed into the first tank at the rate of 100 kg/min and overflows into the second and the third tanks at the same flow rate. The temperature of the oil fed to the first tank is 20°*C*. The tanks are well mixed so that the temperature inside the tanks is uniform, and the outlet stream temperature is the temperature within the tank. The heat capacity, C_p, of the oil is 2.0 KJ/kg. For a particular tank, the rate at which heat is transferred to the oil from the steam coil is given by the expression

$$Q = UA(T_{steam} - T) \tag{18}$$

where UA = 10 kJ/min·°*C* is the product of the heat transfer coefficient and the area of the coil for each tank, T = temperature of the oil in the tank in °*C*, and Q = rate of heat transferred in kJ/min.

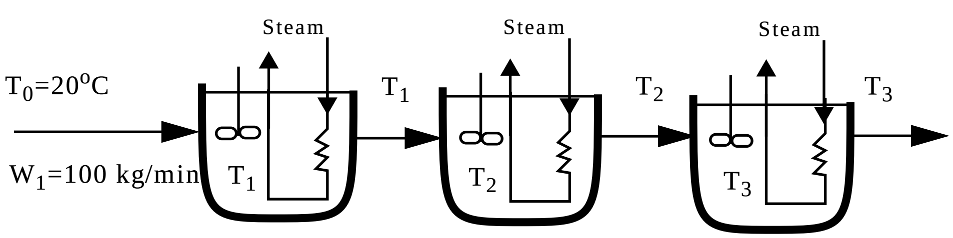

Figure 2 Series of Tanks for Oil Heating

Energy balances can be made on each of the individual tanks. In these balances, the mass flow rate to each tank will remain at the same fixed value. Thus $W = W_1 = W_2 = W_3$. The mass in each tank will be assumed constant as the tank volume and oil density are assumed to be constant. Thus $M = M_1 = M_2 = M_3$. For the first tank, the energy balance can be expressed by

Accumulation = Input - Output

$$MC_p\frac{dT_1}{dt} = WC_pT_0 + UA(T_{steam} - T_1) - WC_pT_1 \tag{19}$$

Note that the unsteady state mass balance is not needed for tank 1 or any other tanks since the mass in each tank does not change with time. The above differential equation can be rearranged and explicitly solved for the derivative which is the usual format for numerical solution.

$$\frac{dT_1}{dt} = [WC_p(T_0 - T_1) + UA(T_{steam} - T_1)]/(MC_p) \tag{20}$$

Similarly for the second tank

$$\frac{dT_2}{dt} = [WC_p(T_1 - T_2) + UA(T_{steam} - T_2)]/(MC_p) \tag{21}$$

For the third tank

$$\frac{dT_3}{dt} = [WC_p(T_2 - T_3) + UA(T_{steam} - T_3)]/(MC_p) \tag{22}$$

Determine the steady state temperatures in all three tanks. What time interval will be required for T_3 to reach 99% of this steady state value during startup?

7. Diffusion with Chemical Reaction in a One Dimensional Slab

7.1 Numerical Methods

Solution of second order ordinary differential equations with two point boundary conditions.

7.2 Concepts Utilized

Methods for solving second order ordinary differential equations with two point boundary values typically used in transport phenomena and reaction kinetics.

7.3 Course Useage

Transport Phenomena and Reaction Engineering.

7.4 Problem Statement

The diffusion and simultaneous first order irreversible chemical reaction in a single phase containing only reactant A and product B results in a second order ordinary differential equation given by

$$\frac{d^2 C_A}{dz^2} = \frac{k}{D_{AB}} C_A \tag{23}$$

where C_A is the concentration of reactant A (kg mol/m^3), z is the distance variable (m), k is the homogeneous reaction rate constant (s^{-1}) and D_{AB} is the binary diffusion coefficient (m^2/s). A typical geometry for Equation (23) is that of a one dimension layer which has its surface exposed to a known concentration and allows no diffusion across its bottom surface. Thus the initial and boundary conditions are

$$C_A = C_{A0} \qquad \text{for } z = 0 \tag{24}$$

$$\frac{dC_A}{dz} = 0 \qquad \text{for } z = L \tag{25}$$

where C_{A0} is the constant concentration at the surface (z = 0) and there is no transport across the bottom surface (z = L) so the derivative is zero.

This differential equation has an analytical solution given by

$$C_A = C_{A0} \frac{\cosh[L(\sqrt{k/D_{AB}})(1 - z/L)]}{\cosh(L\sqrt{k/D_{AB}})} \tag{26}$$

(a) Numerically solve Equation (23) with the boundary conditions of (24) and (25) for the case where C_{A0} = 0.2 kg mol/m^3, $k = 10^{-3}$ s^{-1}, D_{AB} = 1.2 10^{-9} m^2/s, and $L = 10^{-3}$ m. This solution should utilized an ODE solver with a shooting technique and employ Newton's method or some other technique for converging on the boundary condition given by Equation (25).

(b) Compare the concentration profiles over the thickness as predicted by the numerical solution of (a) with the analytical solution of Equation (26).

8. BINARY BATCH DISTILLATION

8.1 Numerical Methods

Solution of a system of equations comprised of ordinary differential equations and nonlinear algebraic equations.

8.2 Concepts Utilized

Batch distillation of an ideal binary mixture.

8.3 Course Useage

Separation Processes.

8.4 Problem Statement

For a binary batch distillation process involving two components designated 1 and 2, the moles of liquid remaining, L, as a function of the mole fraction of the component 2, x_2, can be expressed by the following equation

$$\frac{dL}{dx_2} = \frac{L}{x_2(k_2 - 1)} \qquad \textbf{(27)}$$

where k_2 is the vapor liquid equilibrium ratio for component 2. If the system may be considered ideal, the vapor liquid equilibrium ratio can be calculated from $k_i = P_i/P$ where P_i is the vapor pressure of component i and P is the total pressure.

A common vapor pressure model is the Antoine equation which utilizes three parameters A, B, and C for component i as given below where T is the temperature in °C.

$$P_i = 10^{\left(A - \frac{B}{T + C}\right)} \qquad \textbf{(28)}$$

The temperature in the batch still follow the bubble point curve. The bubble point temperature is defined by the implicit algebraic equation which can be written using the vapor liquid equilibrium ratios as

$$k_1 x_1 + k_2 x_2 = 1 \qquad \textbf{(29)}$$

Consider a binary mixture of benzene (component 1) and toluene (component 2) which is to be considered as ideal. The Antoine equation constants for benzene are A_1 = 6.90565, B_1 = 1211.033 and C_1 = 220.79. For toluene A_2 = 6.95464, B_2 = 1344.8 and C_2 = 219.482 (Dean[1]). P is the pressure in mm

Hg and T the temperature in °C.

The batch distillation of benzene (component 1) and toluene (component 2) mixture is being carried out at a pressure of 1.2 atm. Initially, there are 100 moles of liquid in the still, comprised of 60% benzene and 40% toluene (mole fraction basis). Calculate the amount of liquid remaining in the still when concentration of toluene reaches 80%.

9. REVERSIBLE, EXOTHERMIC, GAS PHASE REACTION IN A CATALYTIC REACTOR

9.1 Numerical Methods

Simultaneous ordinary differential equations with known initial conditions.

9.2 Concepts Utilized

Design of a gas phase catalytic reactor with pressure drop for a first order reversible gas phase reaction.

9.3 Course Useage

Reaction Engineering

9.4 Problem Statement

The elementary gas phase reaction $2A \leftrightarrows C$ is carried out in a packed bed reactor. There is a heat exchanger surrounding the reactor, and there is a pressure drop along the length of the reactor.

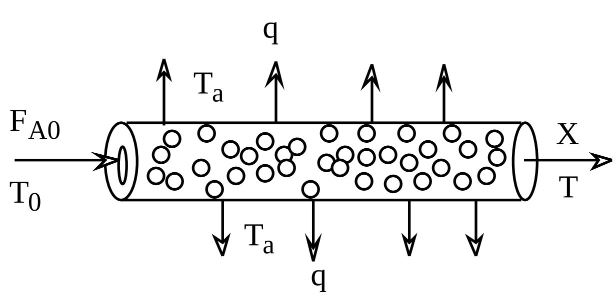

Figure 3 Packed Bed Catalytic Reactor

The various parameters values for this reactor design problem are summarized in Table (3).

Table 3 Parameter Values for Problem 9.

C_{PA} = 40.0 J/g-mol·K	R = 8.314 J/g-mol·K
C_{PC} = 80.0 J/g-mol·K	F_{A0} = 5.0 g-mol/min
ΔH_R = - 40,000 J/g-mol	Ua = 0.8 J/kg·min·K
E_A = 41,800 J/g-mol·K	T_a = 500 K
k = 0.5 dm^6/kg·min·mol @ 450 K	α = 0.015 kg^{-1}
K_C = 25,000 dm^3/g-mol @ 450 K	P_0 = 10 atm
C_{A0} = 0.271 g-mol/dm^3	y_{A0} = 1.0 (Pure A feed)
T_0 = 450 K	

(a) Plot the conversion (X), reduced pressure (y) and temperature ($T \times 10^{-3}$) along the reactor from W = 0 kg up to W = 20 kg.
(b) Around 16 kg of catalyst you will observe a "knee" in the conversion profile. Explain why this knee occurs and what parameters affect the knee.
(c) Plot the concentration profiles for reactant A and product C from W = 0 kg up to W = 20 kg.

Addition Information

The notation used here and the following equations and relationships for this particular problem are adapted from the textbook by Fogler.[2] The problem is to be worked assuming plug flow with no radial gradients of concentrations and temperature at any location within the catalyst bed. The reactor design will use the conversion of A designated by X and the temperature T which are both functions of location within the catalyst bed specified by the catalyst weight W.

The general reactor design expression for a catalytic reaction in terms of conversion is a mole balance on reactant A given by

$$F_{A0}\frac{dX}{dW} = -r'_A \tag{30}$$

The simple catalytic reaction rate expression for this reversible reaction is

$$-r'_A = k\left[C_A^2 - \frac{C_C}{K_C}\right] \tag{31}$$

where the rate constant is based on reactant A and follows the Arrhenius expression

$$k = k(@T{=}450°K)\exp\frac{E_A}{R}\left[\frac{1}{450} - \frac{1}{T}\right] \tag{32}$$

and the equilibrium constant variation with temperature can be determined from van't Hoff's equation with $\Delta\tilde{C}_P = 0$

$$K_C = K_C(@T{=}450°K)\exp\frac{\Delta H_R}{R}\left[\frac{1}{450} - \frac{1}{T}\right] \tag{33}$$

The stoichiometry for $2A \leftrightarrows C$ and the stoichiometric table for a gas allow the concentrations to be expressed as a function of conversion and temperature while allowing for volumetric changes due to decrease in moles during the reaction. Therefore

$$C_A = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{P}{P_0}\frac{T_0}{T} = C_{A0}\left(\frac{1-X}{1-0.5X}\right)y\frac{T_0}{T} \tag{34}$$

and

$$\begin{gathered} y = \frac{P}{P_0} \\ C_C = \left(\frac{0.5C_{A0}X}{1-0.5X}\right)y\frac{T_0}{T} \end{gathered} \tag{35}$$

The pressure drop can be expressed as a differential equation (see Fogler[2] for details)

$$\frac{d\left(\frac{P}{P_0}\right)}{dW} = \frac{-\alpha(1+\varepsilon X)}{2}\frac{P_0}{P}\frac{T}{T_0} \tag{36}$$

or

$$\frac{dy}{dW} = \frac{-\alpha(1-0.5X)}{2y}\frac{T}{T_0} \tag{37}$$

The general energy balance may be written at

$$\frac{dT}{dW} = \frac{U_a(T_a-T)+r'_A(\Delta H_R)}{F_{A0}(\sum \theta_i C_{Pi} + X\Delta\tilde{C}_P)} \tag{38}$$

which for only reactant A in the reactor feed simplifies to

$$\frac{dT}{dW} = \frac{U_a(T_a-T)+r'_A(\Delta H_R)}{F_{A0}(C_{PA})} \tag{39}$$

10. DYNAMICS OF A HEATED TANK WITH PI TEMPERATURE CONTROL

10.1 Numerical Methods

Solution of ordinary differential equations, generation of step functions, simulation of a proportional integral controller.

10.2 Concepts Utilized

Closed loop dynamics of a process including first order lag and dead time. Padé approximation of time delay.

10.3 Course Useage

Process Dynamics and Control

10.4 Problem Statement

A continuous process system consisting of a well-stirred tank, heater and PI temperature controller is depicted in Figure (4). The feed stream of liquid with density of ρ in kg/m^3 and heat capacity of C in kJ / kg·°C flows into the heated tank at a constant rate of W in kg/min and temperature T_i in °C. The volume of the tank is V in m^3. It is desired to heat this stream to a higher set point temperature T_r in °C. The outlet temperature is measured by a thermocouple as T_m in °C, and the required heater input q in kJ/min is adjusted by a PI temperature controller. The control objective is to maintain $T_0 = T_r$ in the presence of a change in inlet temperature T_i which differs from the steady state design temperature of T_{is}.

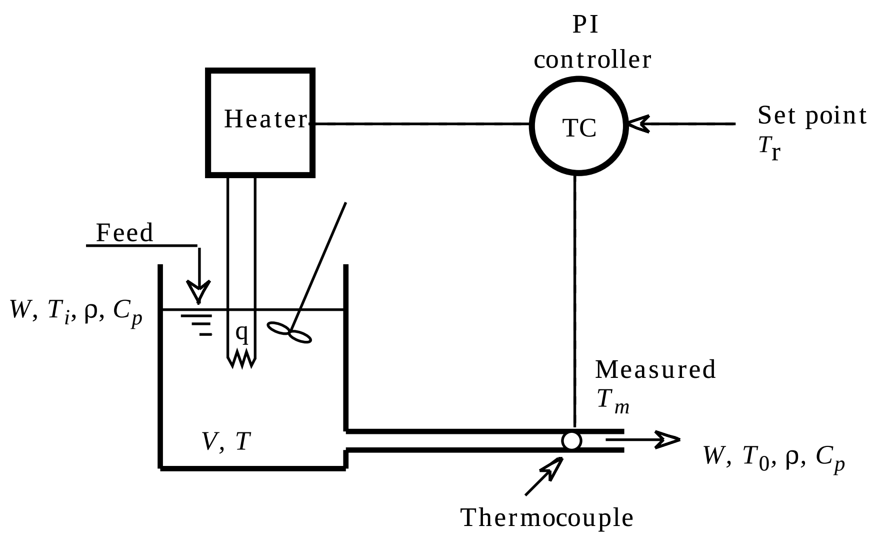

Figure 4 Well Mixed Tank with Heater and Temperature Controller

Modeling and Control Equations

An energy balance on the stirred tank yields

$$\frac{dT}{dt} = \frac{WC_p(T_i - T) + q}{\rho V C_p} \tag{40}$$

with initial condition $T = T_r$ at $t = 0$ which corresponds to steady state operation at the set point temperature T_r.

The thermocouple for temperature sensing in the outlet stream is described by a first order system plus the dead time τ_d which is the time for the output flow to reach the measurement point. The dead time expression is given by

$$T_0(t) = T(t - \tau_d) \tag{41}$$

The effect of dead time may be calculated for this situation by the Padé approximation which is a first order differential equation for the measured temperature.

$$\frac{dT_0}{dt} = \left[T - T_0 - \left(\frac{\tau_d}{2}\right)\left(\frac{dT}{dt}\right)\right]\frac{2}{\tau_d} \qquad \text{I. C. } T_0 = T_r \text{ at } t = 0 \text{ (steady state)} \tag{42}$$

The above equation is used to generated the temperature input to the thermocouple, T_0.

The thermocouple shielding and electronics are modeled by a first order system for the input temperature T_0 given by

$$\frac{dT_m}{dt} = \frac{T_0 - T_m}{\tau_m} \qquad \text{I. C. } T_m = T_r \text{ at } t = 0 \text{ (steady state)} \tag{43}$$

where the thermocouple time constant τ_m is known.

The energy input to the tank, q, as manipulated by the proportional/integral (PI) controller can be described by

$$q = q_s + K_c(T_r - T_m) + \frac{K_c}{\tau_I}\int_0^t (T_r - T_m)dt \tag{44}$$

where K_c is the proportional gain of the controller, τ_I is the integral time constant or reset time. The q_s in the above equation is the energy input required at steady state for the design conditions as calculated by

$$q_s = WC_p(T_r - T_{is}) \tag{45}$$

The integral in Equation (44) can be conveniently be calculated by defining a new variable as

$$\frac{d}{dt}(errsum) = T_r - T_m \qquad \text{I. C. } errsum = 0 \text{ at } t = 0 \text{ (steady state)} \tag{46}$$

Thus Equation (44) becomes

$$q = q_s + K_c(T_r - T_m) + \frac{K_c}{\tau_I}(errsum) \tag{47}$$

Let us consider some of the interesting aspects of this system as it responds to a variety of parameter and operational changes.The numerical values of the system and control parameters in Table (4) will be considered as leading to baseline steady state operation.

Table 4 Baseline System and Control Parameters for Problem 10

$\rho V C_p$ = 4000 kJ/°C	$W C_p$ = 500 kJ/min·°C
T_{is} = 60 °C	T_r = 80 °C
τ_d = 1 min	τ_m = 5 min
K_c = 50 kJ/min·°C	τ_I = 2 min

(a) Demonstrate the open loop performance (set K_c = 0) of this system when the system is initially operating at design steady state at a temperature of 80°C, and inlet temperature T_i is suddenly changed to 40°C at time t = 10 min. Plot the temperatures T, T_0, and T_m to steady state, and verify that Padé approximation for 1 min of dead time given in Equation (42) is working properly.

(b) Demonstrate the closed loop performance of the system for the conditions of part (a) and the baseline parameters from Table (4). Plot temperatures T, T_0, and T_m to steady state.

(c) Repeat part (b) with K_c = 500 kJ/min·°C.

(d) Repeat part (c) for proportional only control action by setting the term K_c/τ_I = 0.

(e) Implement limits on q (as per Equation (47)) so that the maximum is 2.6 times the baseline steady state value and the minimum is zero. Demonstrate the system response from baseline steady state for a proportional only controller when the set point is changed from 80°C to 90°C at t = 10 min. K_c = 5000 kJ/min·°C. Plot q and q_{lim} versus time to steady state to demonstrate the limits. Also plot the temperatures T, T_0, and T_m to steady state to indicate controller performance

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