

5.7

Tank Flow Examples

5.7.1

CONFLO 1, CONFLO 2 and CONFLO 3 – Continuous Flow Tank

System

Liquid flows from an upstream source, at pressure P_1 , via a fixed position valve into the tank, at pressure P_2 . The liquid in the tank discharges via a second fixed position valve to a downstream pressure P_3 . The tank can be open to atmosphere or closed off to the atmosphere and can work either under isothermal or adiabatic temperature conditions. The detailed derivation of this problem is discussed both by Franks (1972) and Ramirez (1976, 1989). Data values in the problem are similar to those of Ramirez, who also presented simulation studies.

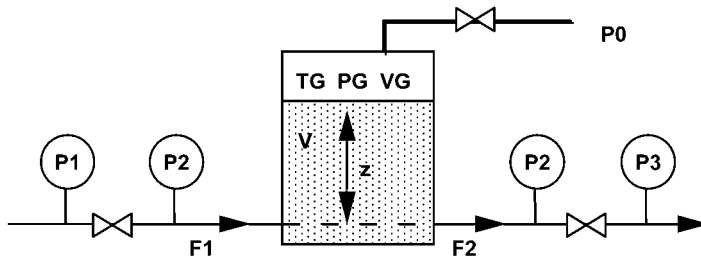


Fig. 1 Schematic of the tank flow problem.

Model

A mass balance for the liquid gives

$$\frac{dM}{dt} = F_1\rho - F_3\rho$$

For constant density ρ

$$\frac{dV}{dt} = A \frac{dz}{dt} = F_1 - F_3$$

where $V = Az$.

The flow through each fixed-position valve is given by

$$F_1 = K_{V1} \sqrt{P_1 - P_2}$$

$$F_3 = K_{V2} \sqrt{P_2 - P_3}$$

where K_{V1} and K_{V2} are the effective valve constants.

Tank pressure and temperature

a) For the tank open to atmosphere, the outlet pressure from the tank P_2 is given by

$$P_2 = P_0 + \rho g z$$

b) For a closed tank under isothermal conditions, the air space above the liquid obeys the Ideal Gas Law

$$PV = nRT$$

so that

$$\frac{P_0 V_G}{T_G} = \frac{P_{G0} V_{G0}}{T_{G0}}$$

where P_{G0} and T_{G0} are the defined initial conditions.

c) Under well insulated conditions, the air in the tank will behave adiabatically and its temperature will change isotropically, where

$$\frac{T_G}{T_{G0}} = \left(\frac{V_{G0}}{V_G} \right)^{\gamma-1}$$

where γ is the adiabatic expansion coefficient for air, equal to 1.4.

Both the upstream pressure P and final downstream pressure P_3 are fixed, together with the atmospheric pressure P_0 .

The above model equations are also presented in dimensionless terms by Ramirez (1989).

Program

The cases (a), (b) and (c) are represented respectively by the simulation programs CONFLO1, CONFLO2 and CONFLO3.

Nomenclature

Symbols

A	Area	m^2
K_V	Valve proportionality factor	$m^4/kN^{0.5} s$

g	Acceleration of gravity	m/s^2
M	Mass	kg
n	Molar mass	kmol
P	Pressure	N/m^2
R	Ideal gas constant	kJm/kmol K
ρ	Density	kg/m^3
T	Temperature	K
V	Volume	m^3
z	Depth of liquid	m
γ	Adiabatic expansion coeff., c_p/c_v	–

Indices

0, 1, 2, 3 Refer to positions (see figures)

Exercises

1. For the open valve case (CONFLO1), make a step change in P_1 and observe the transients in flow rate and liquid level. Try this for a sinusoidally varying inlet pressure. Experiment with a sudden change in the outlet valve setting.
2. For the closed valve case (CONFLO2), repeat the changes of Exercise 1, observing also the variation in the gas pressure and volume. Change the gas volume and note the influence of this variable.
3. Using CONFLO3, determine the importance of including the adiabatic work effects in the model, over a range of flow rate, pressure and valve conditions by following the changes in the gas space temperature and pressure.
4. Study the dimensionless forms of the model equations given by Ramirez (1989); program these and compare the results.

Results

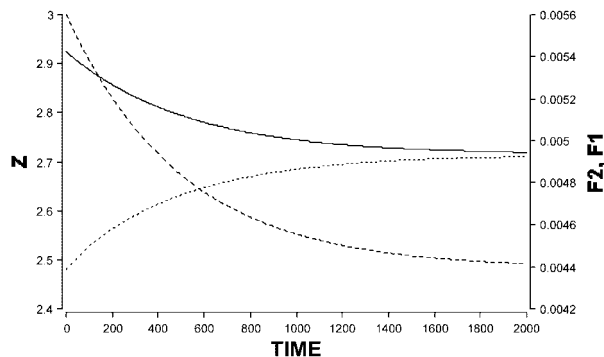


Fig. 2 In CONFLO1, as the liquid height drops the inlet and outlet flows eventually become equal.

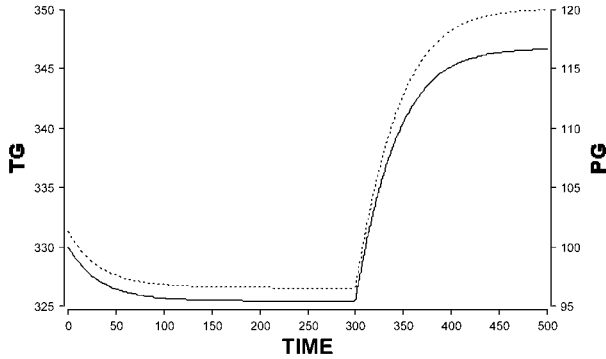


Fig. 3 In CONFLO3, the inlet pressure was changed at time=300 s from 150 to 200 kN/m². Seen here are the temperature and pressure effects of the adiabatic expansion and compression.

References

- Franks, R. G. E. (1972) *Modelling and Simulation in Chemical Engineering*, Wiley-Interscience.
 Ramirez, W. F. (1976) *Process Simulation*, Lexington Books.
 Ramirez, W. F. (1989) *Computational Method for Process Simulation*, Butterworth.

5.7.2

TANKBLD – Liquid Stream Blending

System

Two aqueous streams containing salt at differing concentrations flow continuously into a well-mixed tank, and a mixed-product stream is removed. In this case, the densities of the streams are not assumed constant but vary as a function of concentration. All three streams can have time varying flow rates, and hence the concentration and volume of liquid in the tank will also vary with time.

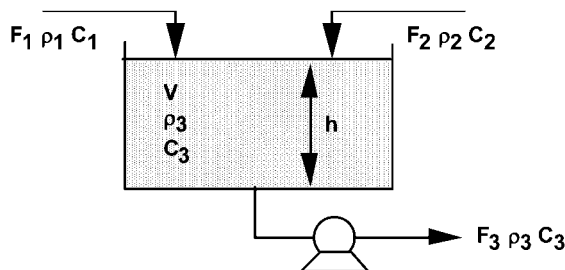


Fig. 1 Tank with density variation.

Model

Total mass balance

$$\frac{d(V\rho_3)}{dt} = F_1\rho_1 + F_2\rho_2 - F_3\rho_3$$

Component mass balance

$$\frac{d(VC_3)}{dt} = F_1C_1 + F_2C_2 - F_3C_3$$

The density of salt solution varies linearly with the concentration of each stream, according to

$$\rho = \rho_0 + bC$$

where b is a constant of proportionality.

The above system was treated in detail by Russell and Denn (1972), and an analytical solution was obtained.

Program

The tank is filled with streams 1 and 2, and when the tank is approximately full, the outlet volumetric flow rate is set to the approximate steady state value, as would be controlled by a pump. This leads to some further volume change as the final product density is reached.

Nomenclature**Symbols**

b	Coefficient in density relation	–
C	Concentration	kg/m^3
F	Volumetric flow rate	m^3/min
V	Volume	m^3
ρ	Density	kg/m^3

Indices

1, 2, 3	Refer to stream values
0	Refers to water

Exercises

1. Carry out simulations for differing tank volumes, flow rates and feed concentrations, in which the inlet and outlet flow rates are set equal ($F_1 + F_2 = F_3$), and observe the approach to steady state. Relate the time taken to approach steady state to the mean tank residence time ($\tau = V/F_3$).
2. Study the case of tank washout, with the tank initially full, at high salt concentration and the liquid input streams free of salt, $C_1 = C_2 = 0$. Show that the tank concentration, C_3 , decreases exponentially with respect to time.
3. Russell and Denn, assuming constant liquid density, showed analytically that

$$C_3 = Z_1 + (C_{30} - Z_1) \left(\frac{1}{1 + Z_2 t} \right)^{Z_3}$$

where

$$Z_1 = \frac{F_1 C_1 + F_2 C_2}{F_1 + F_2}$$

$$Z_2 = \frac{F_1 + F_2 - F_3}{V_0}$$

$$Z_3 = \frac{F_1 + F_2}{F_1 + F_2 - F_3}$$

Here C_{30} is the starting tank concentration at time $t=0$ and V_0 is the starting tank volume at $t=0$. Compare the results of the simulation to the analytical solution which can also be calculated with MADONNA. For the constant density assumption, simply set $b=0$.

The analytical solution shows that the approach to steady state is very rapid when V_0 is small and that the concentration in the tank is always constant, when starting with a relatively empty tank. It also indicates that the rate of change of volume in the tank is equal to the net volumetric flow rate, but only for a linear density concentration relationship. Check the above analytical conclusions numerically and test the case of a non-linear density-concentration relationship by simulation.

4. Modify the program to enable the outlet flow to vary as a function of liquid depth and density, e.g.,

$$F_3 = k\sqrt{\rho_3 V}$$

and test the system with time-varying inlet flows F_1 and F_2 .

Results

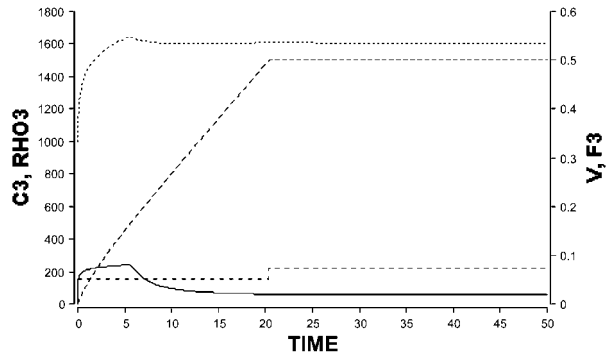


Fig. 2 Variation of C_3 and V during the approach to steady state. Note that V and $RHO3$ continue to change after the final value of F_3 is set.

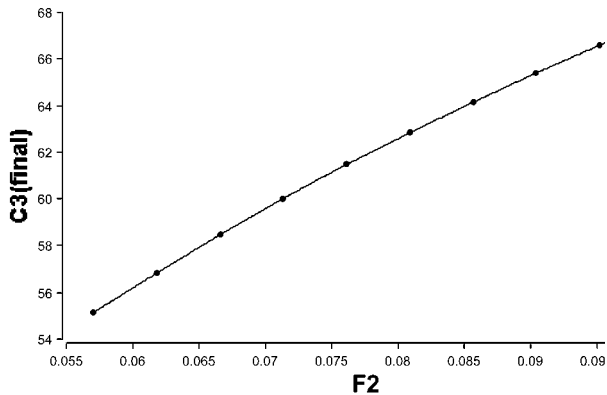


Fig. 3 The steady state values of C_3 as a function of F_2 .

Reference

Russell, T. W. F. and Denn, M. M. (1972) *Introduction to Chemical Engineering Analysis*, Wiley.

5.7.3

TANKDIS – Ladle Discharge Problem

System

The discharge of molten steel from a ladle into a vacuum degassing chamber has been treated by Szekely and Themelis (1971). The transfer is effected via a discharge nozzle, in which the effects of both friction and wear can be important.

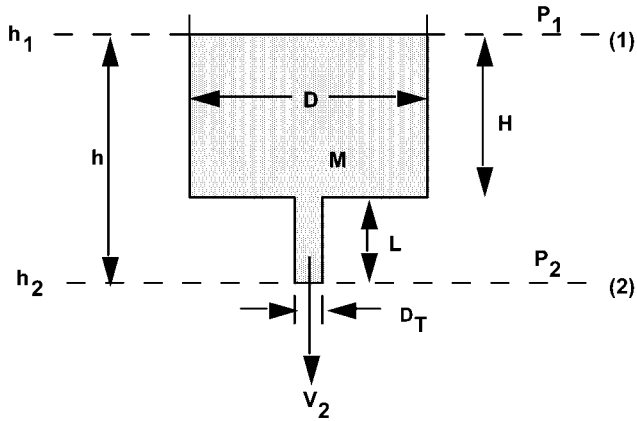


Fig. 1 Schematic drawing of the tank discharge problem.

Model

Total mass balance

$$\frac{dM}{dt} = -W$$

where for the nozzle mass flow

$$W = \frac{\pi D_N^2}{4} \rho v_2$$

For the cylindrical tank geometry the mass as a function of head is

$$M = AH\rho = A\rho(h - L)$$

where $A = (\pi D^2)/4$ and gives the result that

$$h = \frac{M}{A\rho} + L$$

Neglecting acceleration effects in the metal, the energy balance equation is given by

$$\frac{v_1^2}{2g} + h_1 + \frac{P_1}{\rho g} = \frac{v_2^2}{2g} + h_2 + \frac{P_2}{\rho g} + \Delta H_f$$

where ΔH_f represents the losses due to friction and

$$\Delta H_f = \frac{2fLv_2^2}{D_N g}$$

The friction factor, f , depends on the relative surface roughness of the nozzle (ϵ) and the Reynolds number (Re) where

$$Re = \frac{rv_2 D_N}{\mu}$$

A constant value of the friction factor $f=0.009$ is assumed, for fully developed turbulent flow and a relative pipe roughness $\epsilon=0.01$. The assumed constancy of f , however, depends upon the magnitude of the discharge Reynolds number, which is checked during the program. The program also uses the data values given by Szekely and Themelis (1971), but converted to SI units.

Since the velocity of the metal at the ladle surface is very low ($v_1=0$), the metal discharge velocity is then given by

$$v = v_2 = \sqrt{\frac{gh + \frac{P_1 - P_2}{\rho}}{\frac{1}{2} + 2f \frac{L}{D_N}}}$$

Note that a full treatment of this problem would also involve an energy balance and a momentum balance, together with relations for possible physical property changes during discharge and cooling. Acceleration effects are ignored in this analysis, which is solved analytically by Szekely and Themelis.

Nomenclature

Symbols

D	Tank diameter	m
D_N	Nozzle diameter	m
f	Friction factor	–
g	Acceleration of gravity	m/s^2
H	Tank height	m
h	Effective head	m
L	Nozzle length	m
M	Mass	kg
P	Pressure	$kg/m s^2$
ρ	Metal density	kg/m^3
Re	Reynolds number	–
t	time	s
v	Metal velocity	m/s
W	Mass flow rate	kg/s
μ	Metal viscosity	$kg m s$
ΔH_f	Pressure head lost by friction	m

Indices

- 1 Metal surface
- 2 Tank outlet

Exercises

1. Compare the rates of discharge with and without allowance for friction.
2. Modify the program to allow for nozzle wear.
3. How would you expect cooling to affect the discharge rate? How could you make allowance for this in your model?

Results

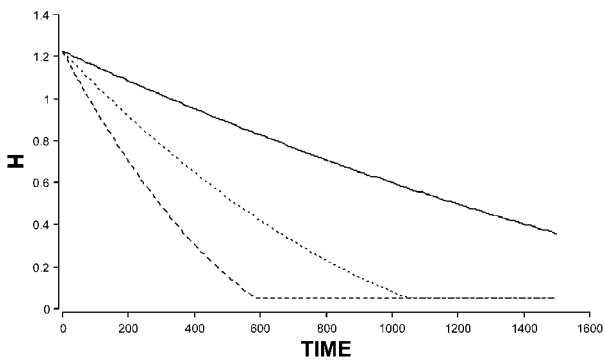


Fig. 2 Liquid level in ladle H as a function of time for three values of the nozzle diameter 0.3 to 0.6 m.

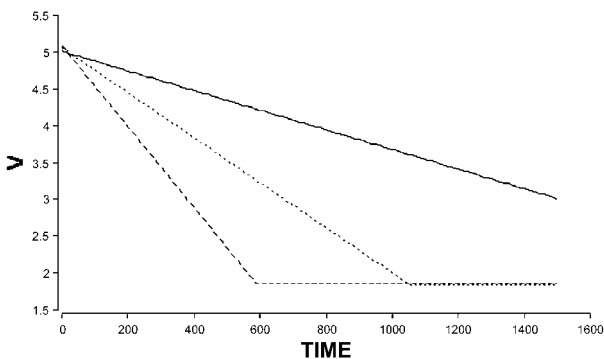


Fig. 3 Discharge velocity as a function of time for three values of the nozzle diameter 0.3 to 0.6 m.

Reference

Szekely, T. and Themelis, N. T. (1971) *Rate Phenomena in Process Metallurgy*, Wiley Interscience.

5.7.4

TANKHYD – Interacting Tank Reservoirs

System

Two open reservoirs with cross-sectional areas A_1 , A_2 and liquid depths h_1 and h_2 are connected by a pipeline of length L and diameter D . The flow of liquid back and forth creates a decaying oscillatory response to a final steady state. Ramirez (1976) provides a detailed model derivation for this problem and shows how the problem is solved by analogue computation. The parameters are the same as those used by Ramirez.

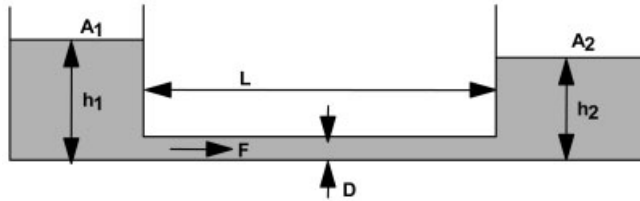


Fig. 1 Dynamics of interacting reservoir levels.

Model

The mass balance for tank 1 at constant liquid density is

$$\frac{d(A_1 h_1)}{dt} = -F$$

and for tank 2

$$\frac{d(A_2 h_2)}{dt} = F$$

where F is the volumetric exchange flow rate between tank 1 and tank 2.

Momentum balance for the pipeline:

$$\left(\begin{array}{c} \text{The rate of} \\ \text{accumulation} \\ \text{of momentum} \end{array} \right) = \left(\begin{array}{c} \text{Rate of} \\ \text{momentum} \\ \text{in} \end{array} \right) - \left(\begin{array}{c} \text{Rate of} \\ \text{momentum} \\ \text{out} \end{array} \right) + \left(\begin{array}{c} \text{Sum of} \\ \text{forces} \\ \text{acting} \end{array} \right)$$

Since the pipeline is of uniform diameter, the rate of momentum at the inlet is equal to that at the outlet and

$$\left(\begin{array}{c} \text{Rate of accumulation} \\ \text{of momentum} \end{array} \right) = \left(\begin{array}{c} \text{Sum of the forces} \\ \text{acting on the pipeline} \end{array} \right)$$

Thus

$$\frac{d(F\rho L)}{dt} = P_1 - P_2 + (-F_x)$$

where P_1 and P_2 are the pressure forces acting on the system

$$P_1 = \frac{\pi D^2}{4} \rho g h_1$$

$$P_2 = \frac{\pi D^2}{4} \rho g h_2$$

and F_x is the frictional force, given by the Fanning frictional equation as

$$F_x = \frac{8F^2}{\pi D^3} f \rho L$$

where f is the Fanning friction factor, assumed constant in this analysis.

Program

Note that the frictional force must always act in the opposite direction to that of the direction of flow and that this must be allowed for in the program.

Nomenclature

Symbols

A	Cross-sectional area of tanks	m^2
D	Diameter of pipe	m
F	Flow rate	m^3/s
f	Overall loss factor	–
F_x	Frictional force	N
g	Acceleration of gravity	m/s^2
h	Liquid depth	m
L	Length of pipe	m
P	Hydrostatic pressure force	N/m^2
t	Time	s
ρ	Liquid density	kg/m^3

Indices

1, 2 Refer to tanks 1 and 2

Exercises

1. Observe the oscillatory approach to steady-state for different initial liquid depths. Plot the depths and the flow rate versus time.
2. Investigate the influence of pipe length and diameter on the time to achieve steady state.
3. Suppose tank 1 represents a body of tidal water with tidal fluctuations, and tank 2 is a tide meter used to measure the height of the tide. The connection is made by 100 m of pipeline and tank 2 is 1 m in diameter. Assume that the tide varies in a sine wave fashion with an amplitude of 2 m with a wave length of 12 h. Change the program to investigate the minimum pipe diameter required to ensure less than a 1 cm difference between the actual tide level and the level in the tide meter.

Results

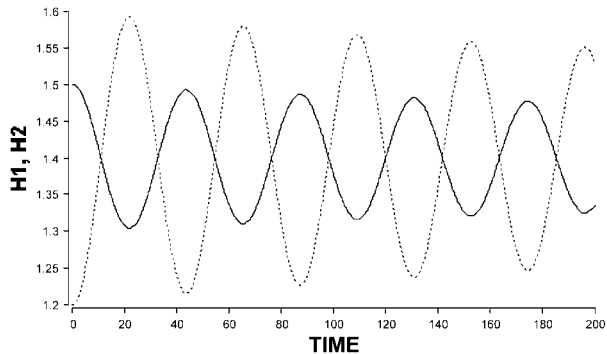


Fig. 2 Oscillating heights of the liquid in the tanks.

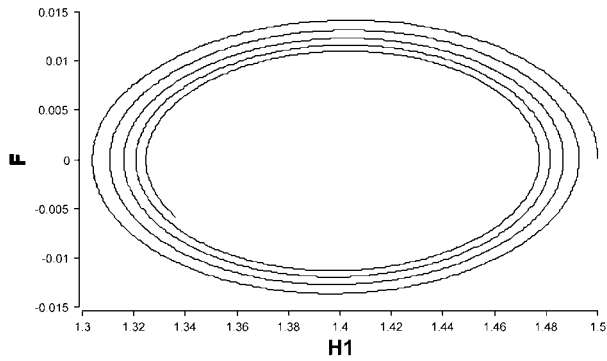


Fig. 3 Phase-plane of liquid height in tank 1 versus flow rate. Note the reversal in the flow direction.

Reference

Ramirez, W.F. (1976) *Process Computation*, Lexington Books.

5.8 Process Control Examples

5.8.1 TEMPCONT – Control of Temperature in a Water Heater

System

The simple feedback control system below consists of a continuous-flow stirred tank, a temperature measurement device, a controller and a heater.

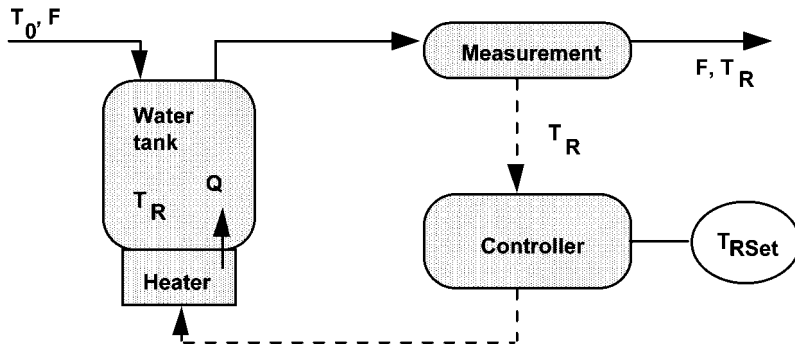


Fig. 1 Feedback control of a simple continuous water heater.

Model

The energy balance for the tank is

$$V \rho c_p \frac{dT_R}{dt} = F \rho c_p (T_0 - T_R) + Q$$

where Q is the delayed heat input from the heater represented by a first order lag

$$\frac{dQ}{dt} = \frac{(Q_c - Q)}{t_Q}$$

The measurement of temperature is also delayed by a sensor lag given by

$$\frac{dT_{\text{sens}}}{dt} = \frac{T_R - T_{\text{sens}}}{\tau_{\text{sens}}}$$

A proportional-integral feedback controller is modelled by

$$Q_c = Q_0 + K_p \varepsilon + \frac{K_p}{\tau_i} \int \varepsilon dt$$

where the control error is given by

$$\varepsilon = (T_{Rset} - T_{sens})$$

Nomenclature

Symbols

c_p	Specific heat	$\text{kJ}/(\text{kg } ^\circ\text{C})$
f	Frequency of oscillations	$1/\text{h}$
F	Flow rate	m^3/h
K_p	Proportional control constant	$\text{kJ}/(\text{h } ^\circ\text{C})$
Q	Heat input	kJ/h
T	Temperature	$^\circ\text{C}$
V	Reactor volume	m^3
ε	Error	$^\circ\text{C}$
ρ	Density	kg/m^3
τ_D	Differential control constant	h
τ_i	Integral control constant	h
τ_Q	Time constant for heater	h
τ_{sens}	Time constant for measurement	h

Indices

C	Refers to controller
R	Refers to reactor
sens	Refers to sensor
set	Refers to setpoint
0	Refers to inlet or initial

Exercises

1. Disconnect the controller (set controller=0), and measure the temperature response to step changes in water flow (set stepflow=1 and steptemp = 0). Observe how the temperature reaches a steady state. From the response curve measure the time constant (63% response)
2. Repeat Exercise 1 for step changes in inlet temperature (set stepflow=0 and steptemp = 1). From the response curve determine T_L and K from the process reaction curve as described in Chapter 2.

3. Measure the controlled response to a step change in F (set controller=1; stepflow=1 steptemp=0) with proportional control only (set τ_I very high). Notice the offset error ε and its sensitivity to K_P . Increase K_P with a small factor, e.g. 1.1, until you observe sustained oscillations. Here it is useful to use the slider tool with a minimum of 1 and a maximum of 1000. Study the influence of K_P on the error ε and the integral of its square, EINT2, using a parameter plot again with logarithmic scale for K_P . Is there any relation between the onset of oscillations and the value of EINT2?
4. Study the influence of the integral part of the controller by changing τ_I to a low value. Does the offset disappear?
5. Referring to Exercise 1, use Cohen–Coon settings from Table 2.2 to obtain the best controller settings for P and PI control from the process reaction curve parameters. Try these out in a simulation. Observe the suitability of the settings from the error e and the integral of its square, EINT2.
6. Operate with proportional control only and a step change in flowrate (set τ_I very high, controller=1; stepflow=1 steptemp=0). Increase K_P until oscillations in the response occur at K_{P0} . Use this oscillation frequency, f_0 , to set the controller according to the Ultimate Gain Method ($K_P=0.45 K_{P0}$, $\tau_I=1/(1.2 f_0)$), where f_0 is the frequency of the oscillations at $K_P=K_{P0}$ (see Sec. 2.3.3). How high is EINT2?
7. Using EINT2 as objective function, vary K_P (KP) and τ_I (TAUI) using the Optimize function in Madonna. Set controller=1; stepflow=1 and steptemp=0. Use parameter plots to verify the minimum.

Results

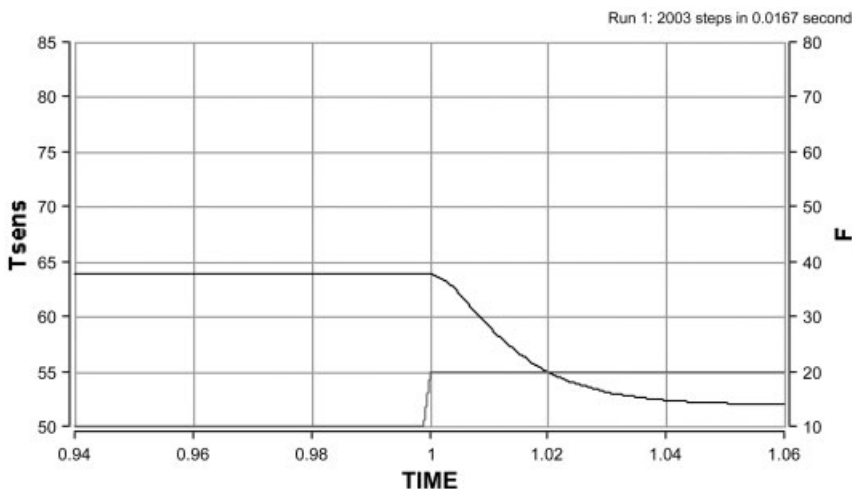


Fig. 2 Response of the system to a step change F as in Exercise 1.

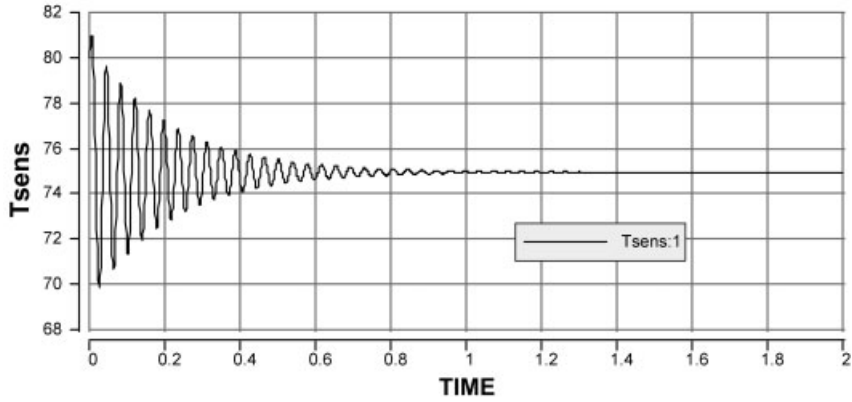


Fig. 3 Response showing damped oscillations at $K_p=290$, as in Exercise 5.

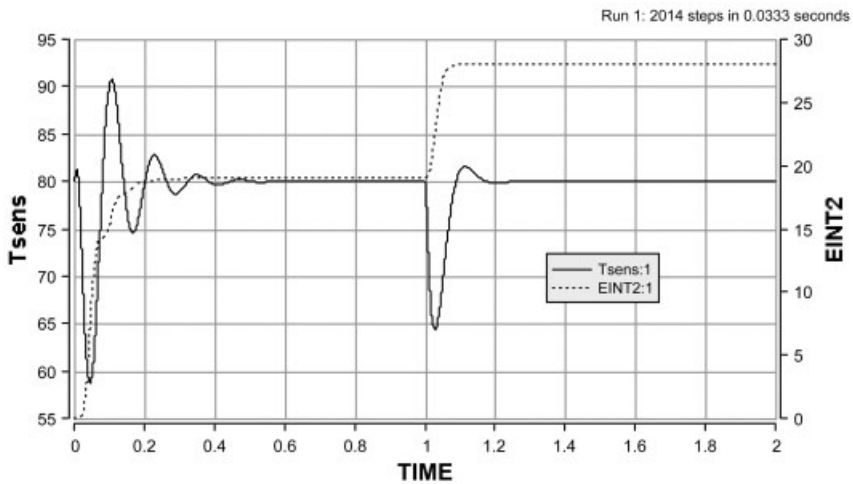


Fig. 4 Response using the control values from the optimisation, as in Exercise 6. Here K_p was limited to a maximum of 10.

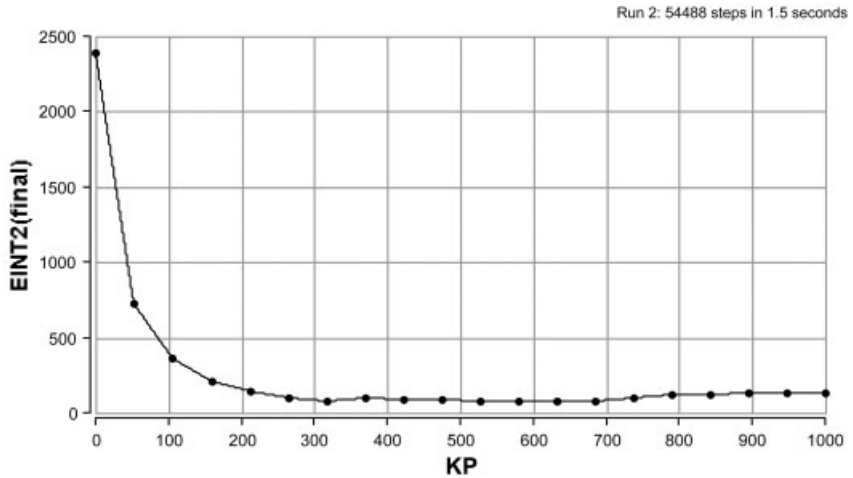


Fig. 5 A parameter plot of K_p showing its influence on $EINT2$.

5.8.2

TWOTANK – Two Tank Level Control

System

Liquid flows through a system of two tanks arranged in series, as shown below. The level control of tank 2 is based on the regulation of the inlet flow to the tank 1. This tank represents a considerable lag in the system. The aim of the controller is to maintain a constant level in tank 2, despite disturbances that occur in the flow F_3 .

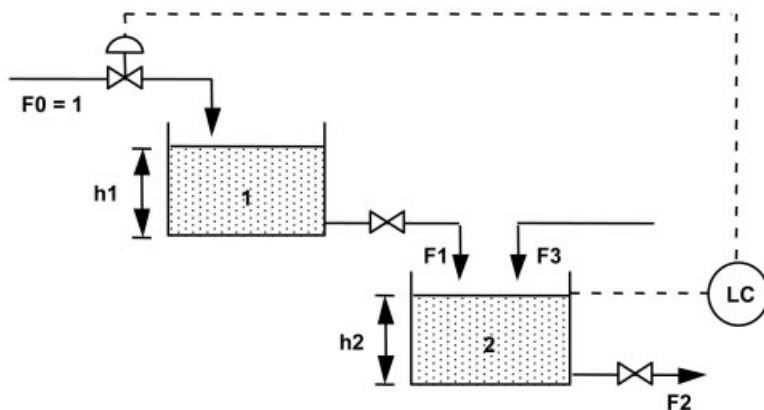


Fig. 1 Level control in a two-tank system.

Model

Mass balance equations with constant density yields
for tank 1

$$A_1 \frac{dh_1}{dt} = F_0 - F_1$$

and for tank 2

$$A_2 \frac{dh_2}{dt} = F_1 + F_3 - F_2$$

Flow equations are given by

$$F_1 = K_1 \sqrt{h_1}$$

$$F_2 = K_2 \sqrt{h_2}$$

The disturbance is generated with a sine wave

$$F_3 = F_{30} + F_{3AMP} \sin \frac{t}{3}$$

and the proportional control equation is

$$F_0 = F_0 + K_p(h_2 - h_{2set})$$

Program

Note the change in the value of the proportional gain KP is changed at 90 h by use of an IF-THEN-ELSE statement:

$$KP = \text{IF TIME} \leq 90 \text{ THEN } 4 \text{ ELSE } 20$$

Nomenclature**Symbols**

A	Tank area	m^2
F	Flow rate	m^3/h
h	Liquid depth	m
K	Valve constant	$m^3/h \ m^{0.5}$
K_p	Controller constant	m^2/h
V	Volume	m^3

Indices

0	Refers to inlet
1	Refers to tank 1
2	Refers to tank 2
3	Refers to feed of tank 2
amp	Refers to amplitude
set	Refers to setpoint

Exercises

1. With no control $K_p=0$ and constant flow of F_3 , study the response of the levels h_1 and h_2 and final steady-state values for differing flow rates F_0 and F_3 .
2. Apply sinusoidal variations in the flow rate F_3 , $F_{3AMP}=0.05$, and again study the responses in h_2 to changes in F_3 .
3. Study the influence of the ratio of A_2/A_1 on the response in h_2 .
4. Set $F_{3AMP}=0$, for constant flow F_3 and study the system response to h_{2set} . Repeat the simulations with control added.
5. Repeat Exercise 3 but with a sinusoidal variation in F_3 , as in Exercise 2.
6. Change the valve constants and note the influence on the dynamics.
7. Change the controller constant and note its influence on the levels and the flow rates.
8. Many other simple combinations of filling and emptying tanks, which can be envisaged and programmed to form the basis of simulation examples.

Results

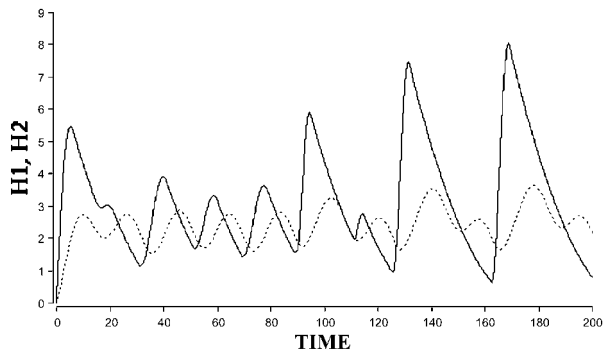


Fig. 2 At $T=90$ the value of the controller constant was increased (K_p from 4 to 20).

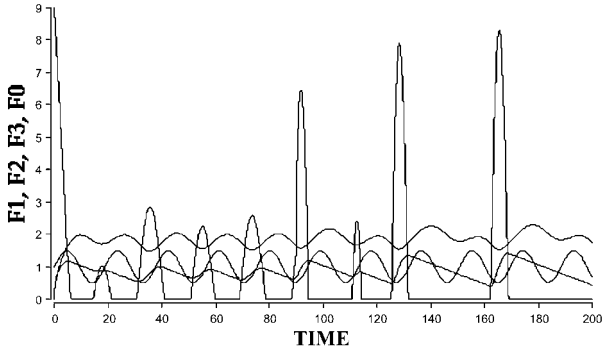


Fig. 3 The increase in K_p at $T=90$ gives very high peaks in F_0 . The sine wave disturbance in F_3 is shown here.

Reference

Smith, C.L. Pike, R. W. and Murril, P. W. (1970) Formulation and Optimisation of Mathematical Models, Intext

5.8.3

CONTUN – Controller Tuning Problem

System

The temperature of a continuous flow of material through a steam-heated stirred tank is controlled by regulating the flow of steam. The tank temperature is measured by a thermocouple set inside a thermowell, giving a delayed temperature measurement response. This example is based on that of Robinson (1975).

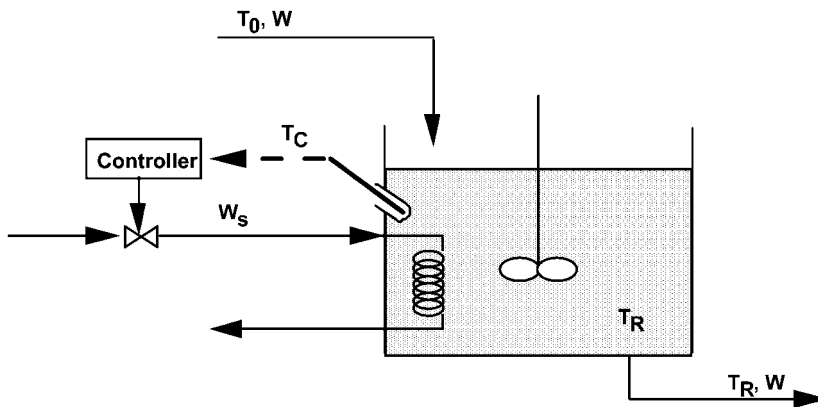


Fig. 1 Tank reactor with control.

Model

Tank heat balance

$$M C_p \frac{dT_R}{dt} = W C_p (T_0 - T_R) + W_S \lambda$$

where λ is the latent heat of the steam entering at the mass flowrate W_S . The temperature of both thermocouple and thermowell are each described by first-order lag equations, so that:

for the thermocouple

$$\frac{dT_C}{dt} = \frac{T_W - T_C}{\tau_C}$$

and for the thermowell

$$\frac{dT_W}{dt} = \frac{T_R - T_W}{\tau_W}$$

where τ_C and τ_W are the lag constants.

Controller Equation

For proportional and integral control

$$W_S = W_{S0} + K_p \varepsilon + \frac{K_p}{\tau_I} \int \varepsilon dt$$

$$\varepsilon = T_{Rset} - T_C$$

Nomenclature**Symbols**

C_p	Specific heat	kJ/kg °C
K_p	Proportional gain	kg/min °C
τ_I	Integral time constant	min
M	Mass	kg
T_R	Temperature of tank	°C
t	Time	min
W	Mass flow rate	kg/min
λ	Latent heat of vapourisation of steam	kJ/kg
τ	Time constant	min

Indices

C	Refers to thermocouple
S	Refers to steam
W	Refers to thermowell
0	Refers to feed condition
I	refers to integral control mode
set	refers to setpoint

Exercises

1. Allow the tank to achieve steady-state operation in the absence of control ($K_p=0$). Use the resulting process reaction curve to estimate combined proportional and integral control parameters. Then use the obtained steady-state values as the initial values for a following sequence of runs.
2. Using proportional control only (τ_I very high), vary the proportional gain constant, in conjunction with a temperature set point change of 10 C and determine the critical value of K_p giving continuous oscillation. Tune the controller for both proportional and integral actions using the Ziegler-Nichols-Criteria, given in Section 2.3.3.2.
3. Experiment with the influence of different values of the measurement time constants, τ_C and τ_W , Plot all the temperatures to compare the results.

Results

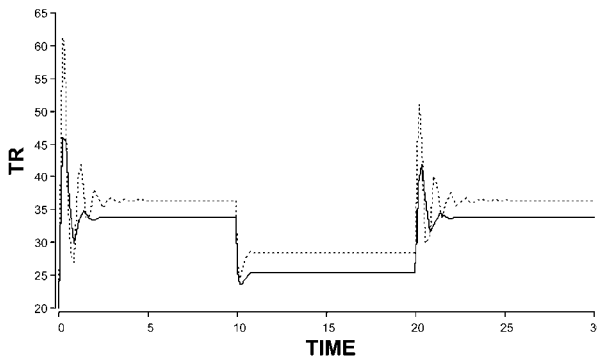


Fig. 2 Tank temperature versus time for two values of K_p (1.5 and 2.0), with $\tau_I=10\,000$. The changes at $T=10$ and $T=20$ are programmed step changes in the inlet water flow rate. Oscillations and offset are caused by sub-optimal controller tuning.

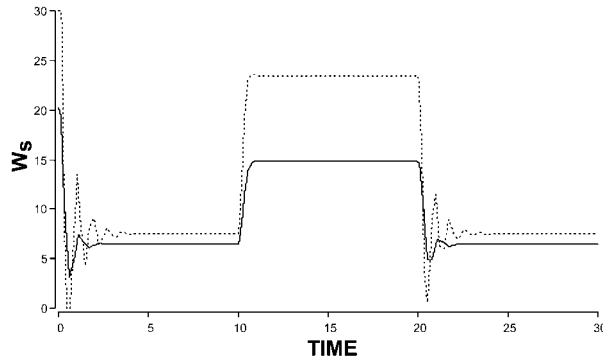


Fig. 3 Variations in steam flow corresponding to the run in Fig. 1.

References

Robinson, E.R. (1975) Time Dependent Processes, Applied Science Publishers.

5.8.4

SEMIEX – Temperature Control for Semi-Batch Reactor

System

An exothermic reaction involving two reactants is run in a semi-continuous reactor. The heat evolution can be controlled by varying the feed rate of one component. This is done via feedback control with reactor temperature measurement used to manipulate the feed rate. The reactor is cooled by a water jacket, for which the heat transfer area varies with volume. Additional control could involve the manipulation of the cooling-water flow rate.

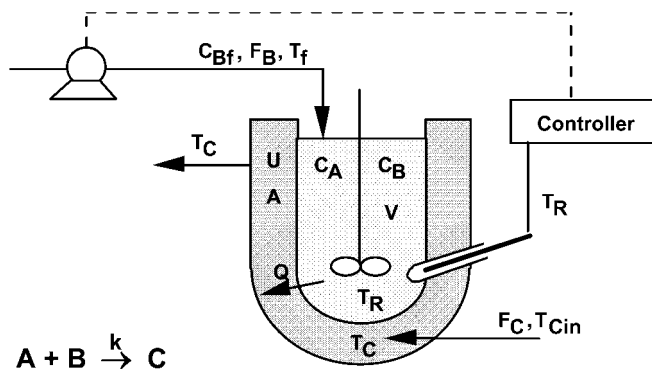


Fig. 1 Exothermic semi-batch reactor with feed control.

Model

The working volume of the reactor is given by the total mass balance, assuming constant density conditions

$$\frac{dV}{dt} = F_B$$

The component balances with second-order kinetics for the variable volume reactor are as follows:

$$\frac{d(V C_A)}{dt} = -k C_A C_B V$$

$$\frac{d(V C_B)}{dt} = F_B C_{Bf} - k C_A C_B V$$

$$\frac{d(V C_C)}{dt} = k C_A C_B V$$

The reaction rate constant varies with absolute temperature as

$$k = k_0 e^{-E/RT_{\text{abs}}}$$

The heat balance for the reactor contents assuming constant physical property values, is

$$V \rho C_p \frac{dT_R}{dt} = F_B \rho C_p (T_f - T_R) - U A (T_R - T_C) + (-\Delta H)(-k C_A C_B V)$$

which simplifies to

$$\frac{dT_R}{dt} = \frac{F}{V} (T_f - T_R) - \frac{U A}{V \rho C_p} (T_R - T_C) + \frac{\Delta H}{\rho C_p} k C_A C_B$$

The cooling jacket is assumed to be well-mixed and is modelled by

$$\rho V_C C_{pc} \frac{dT_C}{dt} = F_C \rho_C C_{pc} (T_{Cin} - T_C) + U A (T_R - T_C)$$

simplifying to

$$\frac{dT_C}{dt} = \frac{F_C}{V_C} (T_{Cin} - T_C) + \frac{U A}{\rho V_C C_{pc}} (T_R - T_C)$$

The level in the tank, h , varies with volume and tank diameter, D , according to

$$h = \frac{V}{\pi(D/2)^2}$$

The heat transfer area changes with liquid level as

$$A = \pi D h$$

The reactor temperature is controlled by manipulating the feed rate according to

$$F_B = F_{B0} + K_p \varepsilon + \frac{K_p}{\tau_I} \int \varepsilon dt$$

where

$$\varepsilon = T_{Rset} - T_R$$

A similar equation could be applied to the manipulation of the cooling water flow.

Program

A partial listing is given below.

{Example SEMIEX}

TRabs=TR+273

d/dt (V) =Fb {Total balance}

A=A0+ (V/C) {Variable transfer area}

k=k0*EXP (-ER/Trabs) {Arrhenius eq.}

{Mass balances}

d/dt (VCa) =-k*Ca*Cb*V

d/dt (VCb) =Fb*CbF-k*V*Ca*Cb

d/dt (VCc) =k*Ca*Cb*V

Ca=VCa/V

Cb=VCb/V

Cc=VCc/V

{Energy balances}

Q=U*A* (TR-TC) / (Rho*Cpr)

d/dt (TR) = (Fb* (Tf-TR) -Q+H*k*Ca*Cb*V / (Rho*Cpr)) /V

d/dt (TC) = (Fc/Vc) * (TCin-TC) +U*A* (TR-TC) / (Rho*Cpc*Vc)

{Feed flow rate control}

Err=TR-Tset

d/dt (Interr) =Err

Fb=Fb0-Kp*Err- (Kp/TI) *Interr

Nomenclature

Symbols

A_0	Initial heat transfer area	m^2
C_A	Concentration of A in tank	$kmol/m^3$
C_{Bf}	Concentration of B fed into tank	$kmol/m^3$
c_p	Heat capacity of reactor and feed	$kJ/kg\ K$
c_{pC}	Heat capacity of cooling water	$kJ/kg\ K$
D	Diameter of tank	m
ER	Activation energy/gas constant, E/R	K
F_{B0}	Feed rate basis	m^3/h
F_C	Cooling water flow	m^3/h
H	Heat of reaction	$kJ/kmol$
h	Level of reactor liquid	m
k	Reaction rate constant	$m^3/kmol\ h$
k_0	Frequency factor	$m^3/kmol\ h$
K_P	Proportional control constant	$m^3/h\ K$
P_i	value of π	–
ρ	Density of all streams	kg/m^3
T_0	Initial temperature in tank	$^\circ C$
T_A	Absolute reactor temperature	K
T_{Cin}	Cooling water temperature	$^\circ C$
T_f	Feed temperature	$^\circ C$
τ_I	Integral control constant	h
T_R and T_{Rabs}	Reactor temperature	$^\circ C$ and K
U	Heat transfer coefficient	$kW/m^2\ K$
V_0	Initial tank volume	m^3
V_C	Volume of cooling jacket	m^3

Indices

abs	Refers to absolute temperature
C	Refers to cooling water
f	Refers to feed values
I	Refers to initial values
in	Refers to cooling water inlet
out	Refers to cooling jacket
set	Refers to setpoint

Exercises

1. Operate the reactor without control using a constant flow of reactant B. Note the reactor temperature.
2. Choose a suitable temperature setpoint and simulate the reactor with control, first with proportional control only and then including integral control. Adjust the controller constants to obtain adequate control.
3. Using the controller constant found in Exercise 2, make a step decrease in the cooling water flow rate. Did the controller decrease the reactant flowrate to compensate for this change?
4. Modify the program and change the controller to manipulate the cooling water flow rate. Experiment with this program.

Results

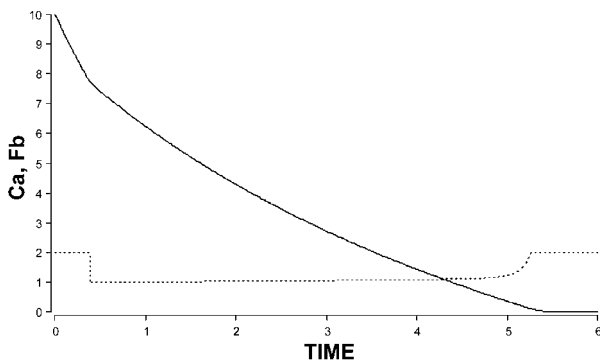


Fig. 2 The feed rate of B, FB, was manipulated by the control equation to control the reactor temperature. At the end of the batch, when the reaction rate decreased due to decreasing CA, FB increased gradually to its maximum.

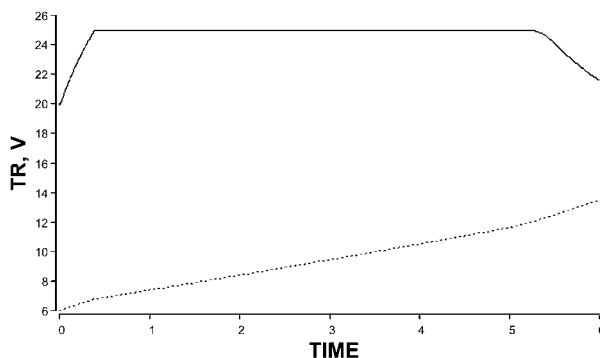


Fig. 3 During the run of Fig. 1, the temperature, TR, at first increased to its setpoint and then decreased at the end of the run. Liquid volume, V, increased throughout the run.

5.8.5

TRANSIM – Transfer Function Simulation**System**

This is based on the example of Matko, Korba and Zupancic (1992), who describe general methods for simulating dynamic systems, when represented in the form of process transform functions. Here the transfer function is given by

$$G(s) = \frac{Y(s)}{U(s)} = \frac{1 - 4s}{(1 + 4s)(1 + 10s)}$$

and this is converted into an equivalent differential equation form for solution by Madonna, via the use of intermediate dummy variables.

Model

The above transfer unit may be written as

$$G(s) = G_1(s)G_2(s)G_3(s)$$

where $G_1(s)$, $G_2(s)$ and $G_3(s)$ relate the outlet response $Y(s)$ to the inlet disturbance $U(s)$, via the assumed dummy variables $W_1(s)$ and $W_2(s)$.

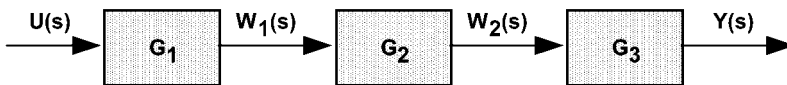


Fig. 1 Transfer function consisting of three transfer functions in series.

Here

$$G_1(s) = \frac{W_1(s)}{U(s)} = \frac{1}{1 + 4s}$$

$$G_2(s) = \frac{W_2(s)}{W_1(s)} = 1 - 4s$$

$$G_3(s) = \frac{Y(s)}{W_2(s)} = \frac{1}{1 + 10s}$$

Hence

$$sW_1 = 0.25U - 0.25W_1$$

$$W_2 = W_1 - 4sW_1$$

$$sY = 0.1W_2 - 0.1Y$$

Defining the variables Y , W_1 and W_2 as deviations from an initial steady state, the original transfer function can now be expressed as

$$\frac{dW_1}{dt} = 0.25U - 0.25W_1$$

$$W_2 = W_1 - 4 \frac{dW_1}{dt}$$

$$\frac{dY}{dt} = 0.1W_2 - 0.1Y$$

Exercises

1. Vary the numerical parameters of the transform and study the resulting response characteristics.
2. Modify the form of the transfer function, convert this into differential equation format and study the resulting response characteristics.
3. Use Madonna to study the response for transfer functions including time delays.

Results

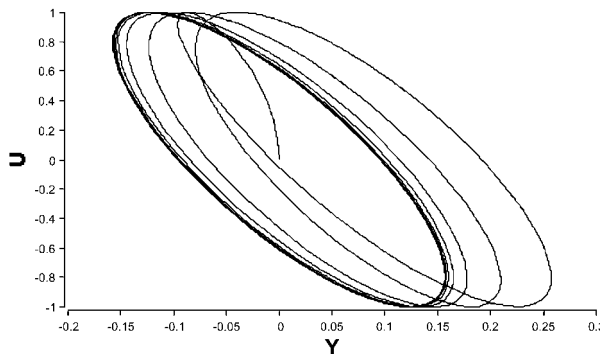


Fig. 2 Phase-plane output for the transfer function with a sine wave disturbance at a frequency of $F=0.1$.

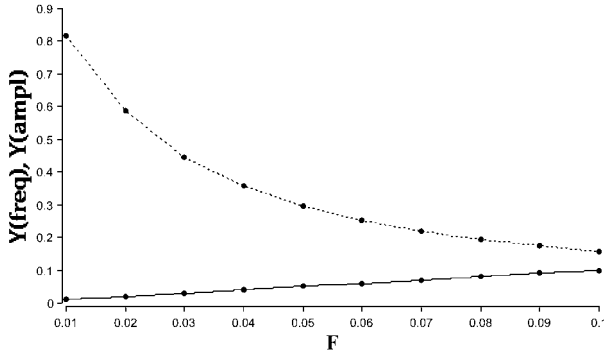


Fig. 3 Varying F from 0.01 to 0.1 in a parametric run that plots automatically the frequency and amplitude of the response.

Reference

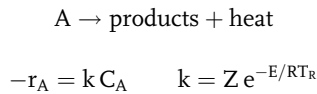
Matko, D., Korba, R. and Zupancic, B. (1992) "Simulation and Modelling of Continuous Systems: A Case Study Approach", Prentice-Hall.

5.8.6

THERMFF – Feedforward Control of an Exothermic CSTR

System

A first-order, exothermic reaction occurs within a continuous stirred-tank reactor, via jacket cooling. The kinetics are given by:



The process model and parameters are the same as in the simulation example THERM.

In this example, the reactor is equipped with a feedforward controller that calculates the flowrate F and the jacket temperature T_j required to maintain the reactor temperature constant for variations in inlet feed concentration C_{A0} and temperature T_0 .

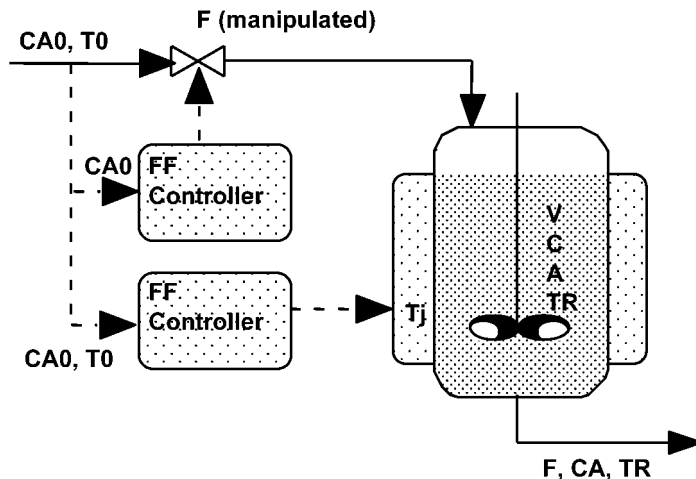


Fig. 1 Feedforward control of a continuous tank reactor with exothermic reaction.

Model

The dynamic process model involves a component balance, energy balance, kinetics and Arrhenius relationship. Hence

$$VT_J = T_R + \frac{C_A k V}{UA} \left(\Delta H + \frac{\rho c_p (T_R - T_0)}{C_{A0} - C_A} \right) = F C_{A0} + F C_A + k V C_A$$

$$V \rho c_p \frac{dT_R}{dt} = F \rho c_p (T_0 - T_R) - k V C_A (-\Delta H) - UA(T_R - T_J)$$

The steady-state forms of these equations allow the manipulation of the feed flowrate F and jacket temperature T_j to maintain the steady state set point under conditions of time-varying C_{A0} and T_0

$$0 = F C_{A0} - F C_A + k V C_A$$

Giving

$$F = \frac{C_A \cdot k V}{C_{A0} - C_A}$$

From this equation the steady state, feed-forward control value of F can be calculated to compensate for variations in C_{A0} with respect to time and based on the setpoint values for k and C_A .

Using the steady state energy balance

$$0 = F \rho c_p (T_0 - T_R) - k V C_A (-\Delta H) - UA(T_R - T_J)$$

C_A may be substituted from the steady state mass balance to give the steady state feed-forward control equation for jacket temperature T_j

$$T_j = T_R + \frac{C_A k V}{U A} \left(\Delta H + \frac{\rho c_p (T_R - T_0)}{C_{A0} - C_A} \right)$$

Note that the values of T_R , C_A , and k are evaluated at the desired setpoint, but that both C_{A0} and T_0 may vary with time as represented here by input sine-wave disturbances.

Programs

The program THERMFF solves the same dynamic process model equations as THERM, where it was shown that all the parameters, including the inlet temperature and concentration will influence the steady state. In the case of multiple steady states the values of the steady state parameters cannot be set, because they are not unique. This example should, therefore, be run under parameter conditions that will guarantee a single steady state for all expected values of the C_{A0} and T_0 . These can be selected with the aid of the programs THERMPLOT and THERM.

Nomenclature

Symbols

c_p	Specific heat	kJ/kg K
ρ	Density	kg/m ³
F	Volumetric feed rate	m ³ /s
V	Reactor volume	m ³
UA	Heat transfer capacity coefficient	kJ/K s
ΔH	Exothermic heat of reaction	kJ/kmol
T	Feed temperature	K
T_R	Reactor temperature	K
C	Concentration	kmol/m ³
Z	Collision frequency	1/s
E	Activation energy	kJ/kmol
R	Gas constant	kJ/kmol K

Indices

0	Refers to feed condition
A	Refers to reactant
J	Refers to jacket

Exercises

1. Using THERMPLOT, vary F to establish a single steady state at the low temperature, low conversion range. With the same parameters, obtain the steady states values of C_A and T_R using THERM. Enter these values as C_{Aset} and T_{Rset} in THERMFF. Using sliders vary the values of F_{min} , T_{Jmin} and T_{Jmax} .
2. Repeat Exercise 1 for a steady state value of high temperature and high conversion.
3. Devise a feedback control loop to correct for any imperfections in the feedforward controller.
4. Investigate the influence of incorrect parameter values in the feedforward control model. Vary the parameters by 10% effects in the control model only to see the effects of uncertainties. This will involve renaming parameters used in the control algorithm, such that the main process parameters still remain the same.

Results

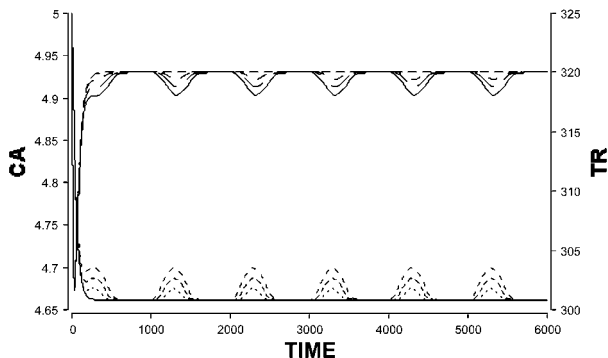


Fig. 2 Reactor response to sine waves in C_{A0} and T_0 under feedforward control, manipulating F and T_j . T_{jmin} was varied from 180 K (perfect control) to 230 K and 260 K

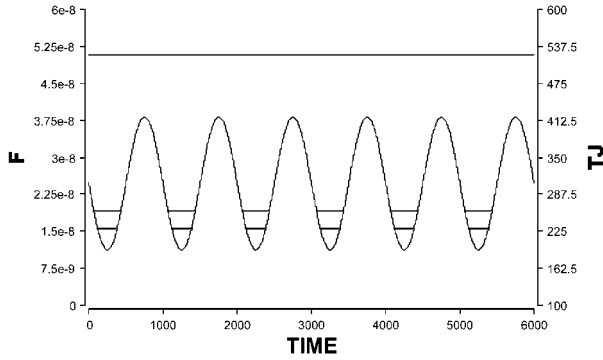


Fig. 3 Manipulated variables showing constant F and T_j variations for the three values of T_{jmin} as in the runs of Fig. 2.

Reference

Luyben, M. L. and Luyben W.L. (1997) *Essentials of Process Control*, McGraw-Hill.

5.9

Mass Transfer Process Examples

5.9.1

BATEX – Single Solute Batch Extraction

System

Consider a batch two-phase extraction system, with a single solute transferring from the feed phase into an immiscible solvent phase. The background to the problem is discussed in Section 3.3.1.1

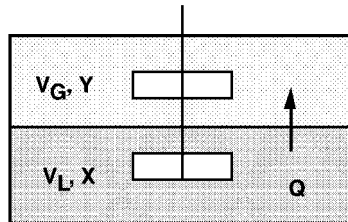


Fig. 1 Batch liquid–liquid extraction.

Solute balances give:

for the feed phase

$$V_L \frac{dX}{dt} = -K_L a (X - X^*) V_L$$

and for the solvent phase

$$V_G \frac{dY}{dt} = +K_L a (X - X^*) V_L$$

where $K_L a$ is the overall mass transfer capacity coefficient (1/s), V_L and V_G are the relative phase volumes (m^3) and where for a linear equilibrium relationship:

$$X^* = \frac{Y}{m}$$

The fractional extraction is given by

$$Z = \frac{X_0 - X}{X_0}$$

where X_0 is the initial charge concentration (kg/m^3).

Program

The program includes a Pulse function, which has been added to the X phase. This is used to represent the effect of sudden addition of solute to this phase at $\text{TIME} = \text{Tswitch}$.

Nomenclature**Symbols**

$K_L a$	Mass transfer capacity coefficient	1/h
m	Equilibrium distribution constant	–
V	Volume	m^3
X	Concentration in X-phase	kg/m^3
Y	Concentration in Y-phase	kg/m^3

Indices

*	Refers to equilibrium
L,G	Refers to L and G phases
0	Refers to the feed condition

Exercises

1. Observe the dynamic approach to equilibrium, and show how the driving force for mass transfer changes with time.
2. Change the value of the mass transfer capacity coefficient $K_L a$ and observe how this affects the time to reach equilibrium. Is there a relationship between $K_L a$ and the system time constant τ ?
3. Vary the value of the equilibrium constant m and study its effect on system behaviour.
4. Study the effect of varying the solvent to feed charge ratio V_L/V_G .
5. Verify that the total mass of solute is conserved.
6. Modify the program to allow for a non-linear equilibrium relationship.

Results

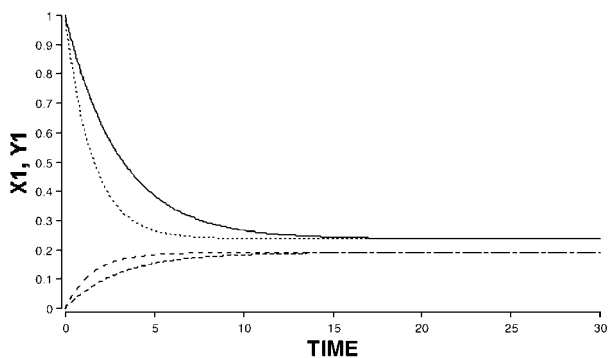


Fig. 2 Dynamic concentration profiles: Effect of $K_La=2.5$ and 5.0 1/h

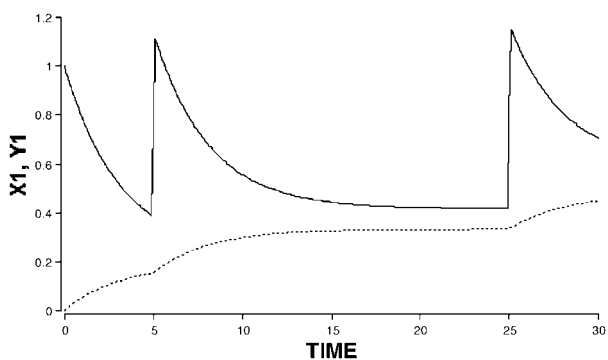


Fig. 3 The X phase is pulsed to suddenly change the concentration.

5.9.2

TWOEX – Two-Solute Batch Extraction with Interacting Equilibria

System

This example considers the interactions involved in multicomponent extraction and takes the particular case of a single batch extractor with two interacting solutes, as shown in Section 3.3.1.2.

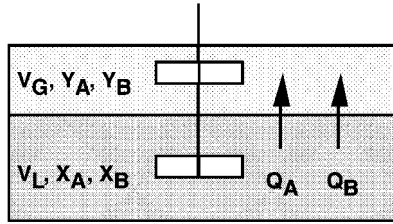


Fig. 1 Batchwise two-solute batch extraction.

Model

Two solutes, A and B, distribute between the feed and solvent phases as concentrations X_A and Y_A , and X_B and Y_B , respectively.

Balances for the two solutes give:

for the feed phase

$$\frac{dX_A}{dt} = -K_{LA}a(X_A - X_A^*)$$

$$\frac{dX_B}{dt} = -K_{LB}a(X_B - X_B^*)$$

and for the solvent phase

$$\frac{dY_A}{dt} = +K_{LA}a(X_A - X_A^*) \frac{V_L}{V_G}$$

$$\frac{dY_B}{dt} = +K_{LB}a(X_B - X_B^*) \frac{V_L}{V_G}$$

The respective equilibrium concentrations, X_A^* and X_B^* , are functions of both solute concentrations, where

$$X_A^* = 1.25Y_A - 0.2Y_B$$

$$X_B^* = Y_B + 0.5Y_A^2$$

Nomenclature

Symbols

V	Phase volume	m^3
X	Solute concentration in the feed phase	kg/m^3
Y	Solute concentration in the solvent phase	kg/m^3
K_{La}	Mass transfer capacity coefficient	$1/h$

Indices

A,B	Solutes A and B
L,G	Feed and solvent phases
*	Equilibrium values

Exercises

1. Observe the influence of the mass transfer capacity coefficients $K_{LA}a$ and $K_{LB}a$ on the system dynamics and on the final approach to equilibrium.
2. Confirm that the total balances for both solutes are correct.
3. Overall mass transfer coefficients are only constant when both liquid film coefficients are constant and also when the slope of the equilibrium line is constant. Thus, for a non-linear equilibrium relationship, the overall mass transfer coefficient will vary with concentration. How would you implement this effect into the program?

Results

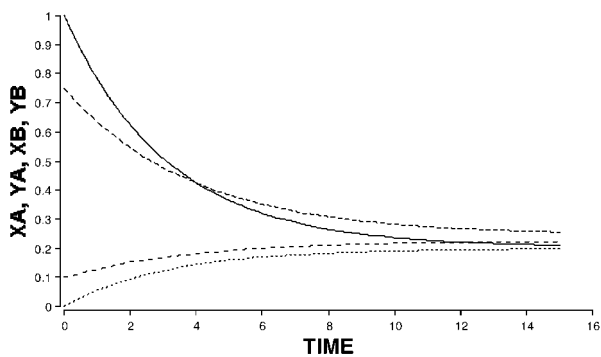


Fig. 2 Time-dependent concentrations for the two-solute extraction.

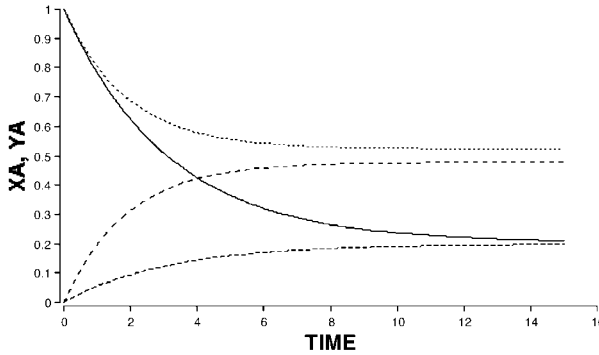


Fig. 3 Time-dependent concentration profiles for solute "A": Effect of phase ratio, with $V_G/V_L = 1.0$ and 4.0 .

5.9.3

EQEX – Simple Equilibrium Stage Extractor

System

This is represented by a single well mixed, constant volume, continuous flow extraction stage.

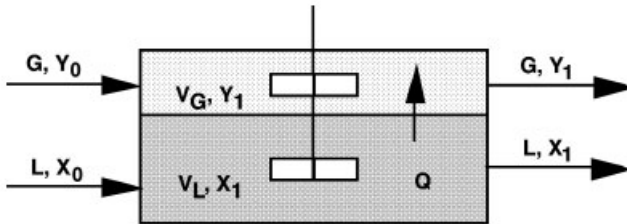


Fig. 1 Continuous equilibrium stage extraction.

Solute balances for each phase give

$$V_L \frac{dX_1}{dt} = LX_0 - LX_1 - K_L a (X_1 - X_1^*) V_L$$

and

$$V_G \frac{dY_1}{dt} = GY_0 - GY_1 + K_L a (X_1 - X_1^*) V_L$$

and where for a linear equilibrium relationship

$$X_1^* = Y_1/m$$

As shown in Section 3.3.1.3, near equilibrium conditions can be obtained by choosing an arbitrarily high value for the mass transfer capacity constant $K_L a$.

Nomenclature

Symbols

G	Flow rate	m^3/h
$K_L a$	Mass transfer capacity constant	$1/h$
L	Flow rate	m^3/h
m	Equilibrium constant	–
V	Volume	m^3
X	Concentration in X-phase	kg/m^3
Y	Concentration in Y-phase	kg/m^3

Indices

*	Refers to equilibrium
0	Refers to inlet
1	Refers to outlet
L,G	Refer to L and G phases

Exercises

1. Vary the system model parameters and see how these affect the time to steady state
2. Compare the residence time for the L phase, V_L/L , with the time constant for mass transfer, $1/K_L a$. Maintain a constant ratio of these two time constants but vary the individual parameters. How is the approach to steady state influenced by these changes?
3. What minimum value of $K_L a$ is required to obtain 99% equilibrium conditions? (Hint – plot X_1 versus X_1^*).

Results

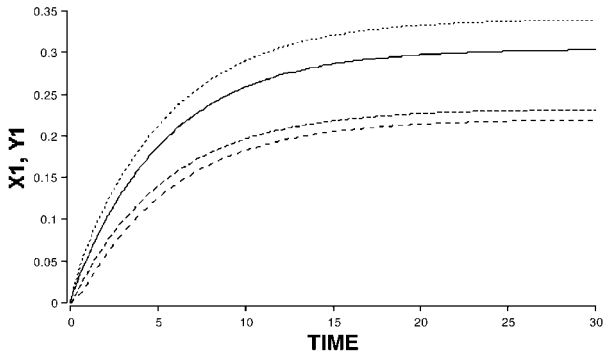


Fig. 2 Approach to steady state [$K_L a = 1$ and 5 1/h]. Note that equilibrium steady state is apparently not attained.

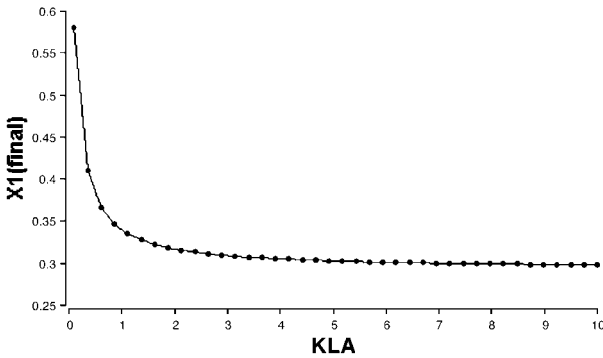


Fig. 3 A parametric run showing that equilibrium conditions are not obtained at low $K_L a$.

5.9.4

EQMULTI – Continuous Equilibrium Multistage Extraction

System

A countercurrent multistage extraction system is to be modelled as a cascade of equilibrium stages.

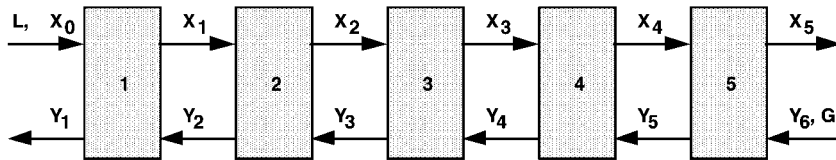


Fig. 1 Countercurrent multistage equilibrium extraction unit.

Model

The solute balances for any stage n are given by

$$V_L \frac{dX_n}{dt} = L(X_{n-1} - X_n) - Q_n$$

$$V_G \frac{dY_n}{dt} = G(Y_{n+1} - Y_n) + Q_n$$

where

$$Q_n = K_L a (X_n - X_n^*) V_L$$

and for a linear equilibrium

$$X_n^* = Y_n/m$$

As in example EQEX, the mass transfer capacity coefficient $K_L a$ may be set high to obtain near equilibrium stage conditions.

Program

Note that the program is written such that the number of stages in the cascade, N_{stage} , can be varied as an additional parameter in the simulation. The stage numbers can be plotted versus the final values by choosing $[i]$ as the X-axis. In this way the steady state concentration profiles can be graphed. A part of the program is shown below.

```
{Example EQMULTI}
INIT X [1..Nstage]=0
INIT Y [1..Nstage]=0

{Mass transfer rates kg/h}
Q [1..Nstage]=KLa*(X[i]-Y[i]/M)*VL
```

```

{Component balances for stage 1}
d/dt (X[1]) = (L*X0 - L*X[1] - Q[1]) / VL
d/dt (Y[1]) = (G*(Y[2] - Y[1]) + Q[1]) / VG

{Extract outlet concentration}
Y1= Y[1]

{Component balances for stages 2 to Nstage-1}
d/dt (X[2..Nstage-1]) = (L*(X[i-1] - X[i]) - Q[i]) / VL
d/dt (Y[2..Nstage-1]) = (G*(Y[i+1] - Y[i]) + Q[i]) / VG

{Component balances for stage Nstage}
d/dt (X[Nstage]) = (L*(X[i-1] - X[i]) - Q[i]) / VL
d/dt (Y[Nstage]) = (G*YNstage - G*Y[i] + Q[i]) / VG

{Raffinate outlet concentration}
YN= Y[Nstage]

```

Nomenclature

Symbols

G	Flow rate	m^3/h
$K_{L,a}$	Mass transfer capacity constant	$1/\text{h}$
L	Flow rate	m^3/h
m	Equilibrium constant	–
Q	Solute transfer rate	kg/h
V	Volume	m^3
X_1	Concentration in X-phase	kg/m^3
Y_1	Concentration in Y-phase	kg/m^3

Indices

*	Refers to equilibrium
0	Refers to inlet
L,G	Refer to L and G phases
n	Refers to stage

Exercises

1. Run the model for the 5-stage model and ascertain if equilibrium is attained for each stage. Reduce $K_{L,a}$ by a factor of 10 and check again. Reduce L and G by the same factor. Explain the effects in terms of the process time constants.
2. Confirm that the overall solute balance is satisfied at steady state.
3. Carry out further simulations on the model and investigate the number of stages required for say 99% separation recovery as a function of the other system parameters.

4. Modify the above program to model the case of a discontinuous five-stage extraction cascade, in which a continuous flow of aqueous phase L is passed through the cascade. The solvent is continuously recycled through the cascade and also through a solvent holding tank, of volume V_S , as shown below. This problem of a stagewise discontinuous extraction process has been solved analytically by Lelli (1966).
5. Try to predict the form of the L and G phase responses before carrying out simulations for the above problem.
6. Vary L and G and observe the influence on the dynamics. Explain the results in terms of the system time constants.

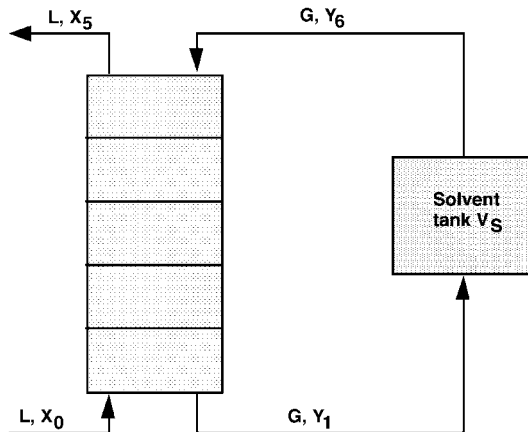


Fig. 2 Modification of EQMULTI with recycle of solvent.

Results

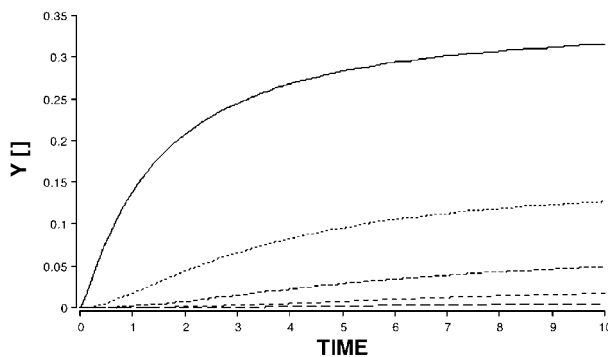


Fig. 3 Approach to near steady state for the L phase solute concentrations.

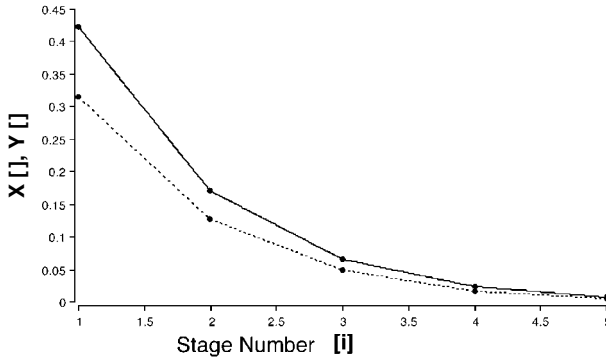


Fig. 4 Near steady state concentration profiles showing almost complete extraction to have been obtained.

Reference

Lelli, U. (1966) *Annali di Chimica* 56, 113.

5.9.5

EQBACK – Multistage Extractor with Backmixing

System

The full model is described in Section 3.3.1.5 and consists of a countercurrent stagewise extraction cascade with backmixing in both phases.

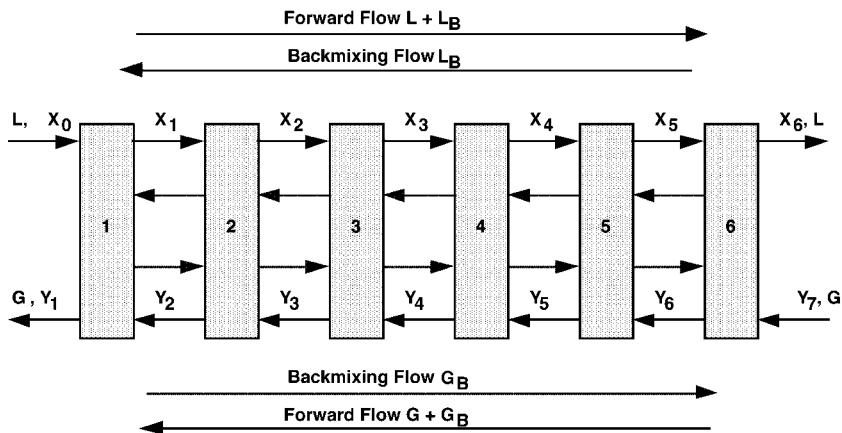


Fig. 1 Multistage extractor with backmixing.

Model

Allowing for the backmixing flow contributions, the continuity equations for any stage n are

$$V_L \frac{dX_n}{dt} = (L + L_B)(X_{n-1} - X_n) + L_B(X_{n+1} - X_n) - Q_n$$

$$V_G \frac{dY_n}{dt} = (G + G_B)(Y_{n+1} - Y_n) + G_B(Y_{n-1} - Y_n) + Q_n$$

where $Q_n = K_L a(X_n - X_n^*)V_L$ and $X_n^* = Y_n/m$

The model equations are also often written in terms of backmixing factors, where

$$a_L = L_B/L \quad \text{and} \quad a_G = G_B/G$$

Special balances also apply to the end sections owing to the absence of back-flow, exterior to the column.

Nomenclature**Symbols**

a	Backmixing factor	–
G	Flow rate	m^3/h
$K_L a$	Mass transfer capacity coefficient	$1/\text{h}$
L	Flow rate	m^3/h
m	Equilibrium constant	–
Q	Transfer rate	kg/h
V	Volume	m^3
X	Concentration in X-phase	kg/m^3
Y	Concentration in Y-phase	kg/m^3

Indices

*	Refers to equilibrium
0	Refers to inlet
L,G	Refer to L and G phases
B	Refers to backmixing
n	Refers to stage number

Program

Note that the program is written such that the number of stages in the cascade may be used an additional parameter in the simulation.

Exercises

1. Vary the backmixing flows for each phase and notice the effect of changes in conditions between plug flow and full backmixing on the performance of the extractor.
2. For which conditions of backmixing does the extraction process operate best?
3. Check the steady-state overall solute balances.

Results

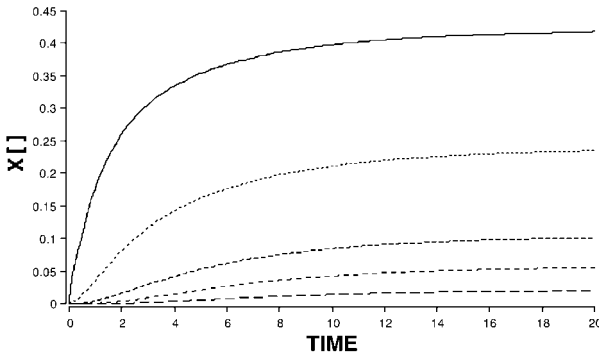


Fig. 2 Time-dependent concentrations for the feed phase in stages 1 to 5 [$a_L=0.15$ and $a_C=0.15$].

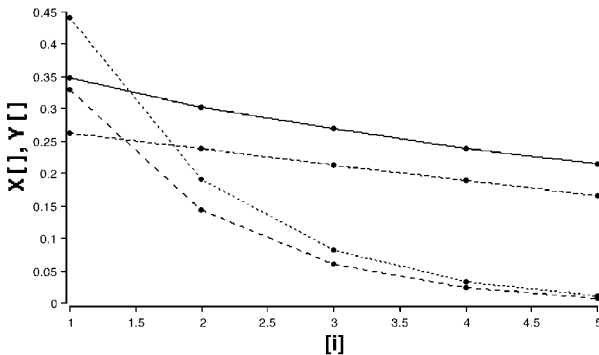


Fig. 3 High backmixing [$a_L=5$, $a_C=5$] flattens the steady state concentration profiles and therefore reduces extraction efficiency, as compared to zero backmixing conditions [$a_L=0$, $a_C=0$], as seen in this axial profile plot.

5.9.6

EXTRACTCON – Extraction Cascade with Backmixing and Control**System**

In this example of a five stage extraction column with backmixing, proportional plus integral control of the exit raffinate concentration is to be achieved by regulating solvent flowrate.

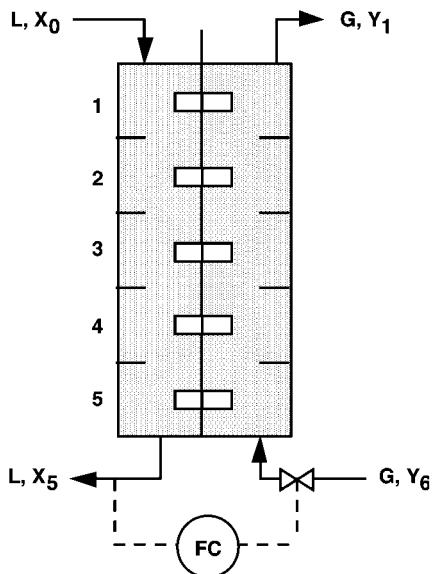


Fig. 1 Five stage extraction cascade with control.

Model

The solute balance equations for each phase are

$$V_L \frac{dX_n}{dt} = (L + L_B)(X_{n-1} - X_n) + L_B(X_{n+1} - X_n) - Q_n$$

$$V_G \frac{dY_n}{dt} = (G + G_B)(Y_{n+1} - Y_n) + G_B(Y_{n-1} - Y_n) + Q_n$$

where

$$Q_n = K_L a (X_n - X_n^*) V_L \quad \text{and} \quad X_n^* = Y_n / m$$

The PI controller equation is

$$G = G_0 + K_C \varepsilon + \frac{K_C}{\tau_I} \int \varepsilon dt$$

where

$$\varepsilon = X_n - X_{n \text{ set}}$$

and $X_{n \text{ set}}$ is the controller set point.

Program

The simulation starts from initially zero concentration conditions along the cascade. Control is implemented from time $t=0$, in order to obtain an outlet raffinate concentration equal to the controller set point. The program is essentially the same as that used in EQBACK, but with added controller equations.

Nomenclature

Symbols

G	Flow rate	m^3/h
G_0	Base solvent flow rate	m^3/h
K_C	Proportional control constant	$(\text{m}^3/\text{hr})/(\text{kg}/\text{m}^3)$
$K_{L,a}$	Mass transfer capacity coefficient	$1/\text{h}$
L	Flow rate	m^3/h
m	Equilibrium constant	–
Q	Transfer rate	kg/h
V	Phase volume	m^3
X	Concentration in X-phase	kg/m^3
X_{SET}	Raffinate concentration setpoint	kg/m^3
Y	Concentration in Y-phase	kg/m^3
ε	Controller error	kg/m^3
τ_I	Integral control time constant	h

Indices

*	Refers to equilibrium
0	Refers to inlet
L,G	Refer to L and G phases
B	Refers to backmixing
n	Refers to stage number

Exercises

1. Study the response of the system with only proportional control (τ_I very large) and determine the resultant steady state offset. Add an increasing degree of integral control and study its effect.
2. Try tuning the controller to obtain the best response to a change in feed concentration and feed rate.
3. Set the initial concentration profiles in the two phases equal to the steady state open loop response ($K_C = 0$), and study the response of the system to another set point change or flow rate change.

Results

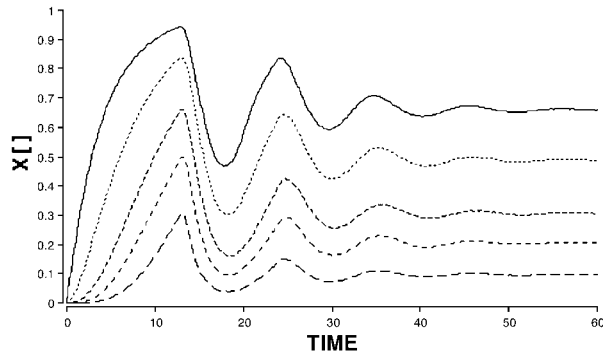


Fig. 2 Concentration variations in the feed phase for stages 1 to 5 and for start up from initially zero concentration conditions with full control implementation ($K_C=5$).

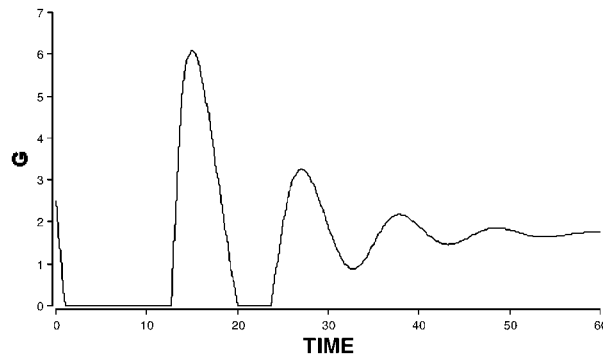


Fig. 3 The corresponding solvent flow variations.

5.9.7

HOLDUP – Transient Holdup Profiles in an Agitated Extractor**System**

The fractional holdup of the dispersed phase in agitated extraction columns varies as a function of flowrate. Under some circumstances it may be important to model the corresponding hydrodynamic effect. The system is represented below as a column containing seven agitated compartments or stages.

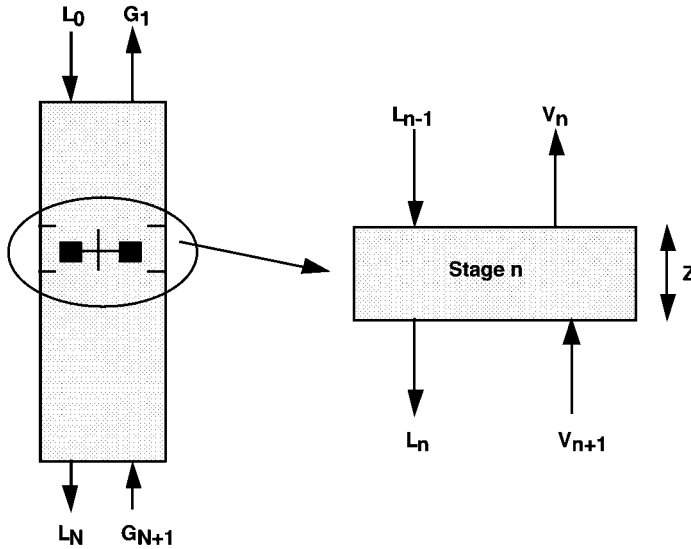


Fig. 1 Seven-stage agitated column contactor.

Model

The variation in the holdup of solvent dispersed phase is given by

$$V_n \frac{dh_n}{dt} = G_{n+1} - G_n$$

Since the two liquid phases are also incompressible, then

$$L_{n-1} + G_{n+1} = L_n + G_n$$

and for the overall column

$$L_0 + G_{N+1} = L_N + G_1$$

In this example, it is assumed that the holdup relationship is given as a direct empirical function of the continuous and dispersed phase flow rates. This avoids any difficulties due to a possible algebraic implicit loop in the solution (see Section 3.3.1.11).

For a given range of feed flow rate, L , it is assumed that the fractional holdup, h , and the solvent phase flow rate, G , can be correlated in the form

$$G = h^{a/b}$$

where “ a ” and “ b ” are empirical constants and the flow rates are expressed as superficial phase velocities.

Program

The program is written in array form, with N_{cmpts} the parameter representing the desired number of compartments in the column. The simulation starts with a uniform holdup distribution throughout the column and with the column operating at steady-state. At time, T_{switch} , the organic solvent flow is suddenly increased, as effected by the use of a MADONNA IF-THEN-ELSE command.

Nomenclature

Symbols

a, b	Holdup relation parameters	
G	Organic, dispersed phase flow velocity	$\text{cm}^3 / \text{cm}^2 \text{ h}$
h	Fractional holdup of dispersed phase	–
L	Aqueous, continuous phase flow velocity	$\text{cm}^3 / \text{cm}^2 \text{ h}$
N_{cmpts}	Compartment number	–
t	Time	h
T_{switch}	Switching time	h
V	Volume	cm^3

Index

n	Compartment number
-----	--------------------

Exercises

1. Vary the holdup parameters a and b to study their effect on the resulting holdup variations.
2. The holdup changes are the result of interdroplet interactions, which may also have their own dynamics. Assume that this can be represented by a first order lag equation, and show how this effect may be implemented into the simulation.
3. An important limit to extraction column behaviour is of course that of column flooding. How could this effect also be incorporated into the simulation?

Results

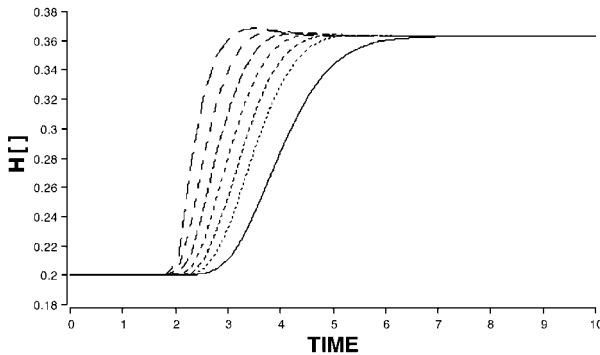


Fig. 2 Holdup response to an increase in organic (dispersed) phase flow.

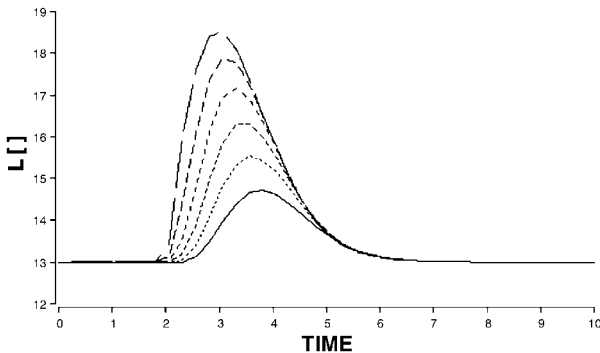


Fig. 3 Response of the continuous aqueous phase flow rates for the Fig. 2 run.

5.9.8

KLADYN, KLAFIT and ELECTFIT – Dynamic Oxygen Electrode Method for $K_L a$

System

A simple and effective means of measuring the oxygen transfer coefficient ($K_L a$) in an air-water tank contacting system involves first degassing the batch water phase with nitrogen (Ruchti et al., 1981). Then the air flow is started and the increasing dissolved oxygen concentration is measured by means of an oxygen electrode.

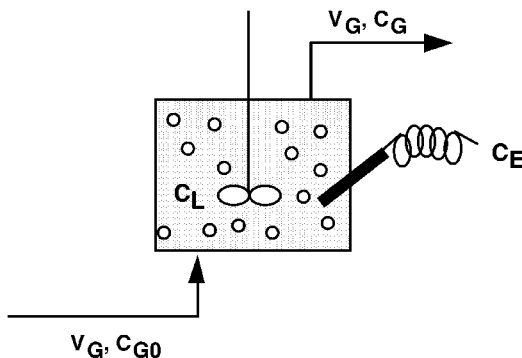


Fig. 1 Aerated tank with oxygen electrode.

As shown below, the influence of three quite distinct dynamic processes plays a role in the overall measured oxygen concentration response curve. These are the processes of the dilution of nitrogen gas with air, the gas-liquid transfer and the electrode response characteristic, respectively. Whether all of these processes need to be taken into account when calculating $K_L a$ can be determined by examining the mathematical model and carrying out simulations.

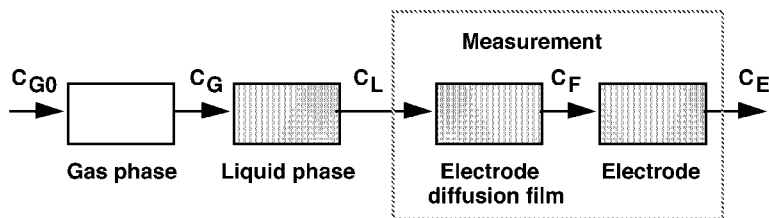


Fig. 2 Representation of the process dynamics.

Model

The model relationships include the mass balance equations for the gas and liquid phases and equations representing the measurement dynamics.

Oxygen Balances

The oxygen balance for the well-mixed flowing gas phase is described by

$$V_G \frac{dC_G}{dt} = G(C_{G0} - C_G) - K_L a (C_L^* - C_L) V_L$$

where $V_G/V = \tau_G$ and $K_L a$ is based on the liquid volume.

The oxygen balance for the well-mixed batch liquid phase is

$$V_L \frac{dC_L}{dt} = K_L a (C_L^* - C_L) V_L$$

The equilibrium oxygen concentration C_L^* is given by the combination of Henry's law and the Ideal Gas Law equation where

$$C_L^* = \frac{RT}{H} C_G$$

and C_L^* is the oxygen concentration in equilibrium with the gas concentration C_G . The above equations can be solved in this form as in simulation example KLAFIT. It is also useful to solve the equations in dimensionless form.

Oxygen Electrode Dynamic Model

The response of the usual membrane-covered electrodes can be described by an empirical second-order lag equation. This consists of two first-order lag equations to represent the diffusion of oxygen through the liquid film on the surface of the electrode membrane and secondly the response of the membrane and electrolyte:

$$\frac{dC_F}{dt} = \frac{C_L - C_F}{\tau_F}$$

and

$$\frac{dC_E}{dt} = \frac{C_F - C_E}{\tau_E}$$

τ_F and τ_G are the time constants for the film and electrode lags, respectively. In non-viscous water phases τ_F can be expected to be very small and the first lag equation can, in fact, be ignored.

Dimensionless Model Equations

Defining dimensionless variables as

$$C'_G = \frac{C_G}{D_{G0}} \quad C'_L = \frac{C_L}{C_{G0}(RT/H)} \quad t' = \frac{t}{\tau_G}$$

the component balance equations then become

$$\frac{C'_G}{dt'} = (1 - C'_G) - K_L a \tau_G \frac{V_L}{V_G} \frac{RT}{H} (C'_G - C'_L)$$

and

$$\frac{C'_L}{dt'} = K_L a \tau_G (C'_G - C'_L)$$

Initial conditions corresponding to the experimental method are

$$t' = 0; \quad C'_L = C'_G = 0$$

In dimensionless form the electrode dynamic equations are

$$\frac{dC'_F}{dt'} = \frac{C'_L - C'_F}{\tau_F/\tau_G}$$

and

$$\frac{dC'_E}{dt'} = \frac{C'_F - C'_E}{\tau_E/\tau_G}$$

where C'_F is the dimensionless diffusion film concentration.

$$\frac{C_F}{C_{G0}(RT/H)}$$

and C'_E is the dimensionless electrode output

$$\frac{C_E}{C_{G0}(RT/H)}$$

As shown by Dang et al. (1977), solving the model equations by Laplace transformation gives

$$a = \frac{1}{K_L a} + \left(\frac{RT}{H} \frac{V_L}{V_G} + 1 \right) \tau_G + \tau_E + \tau_F$$

where a is the area above the C'_E versus t response curve, as shown in Fig. 3.

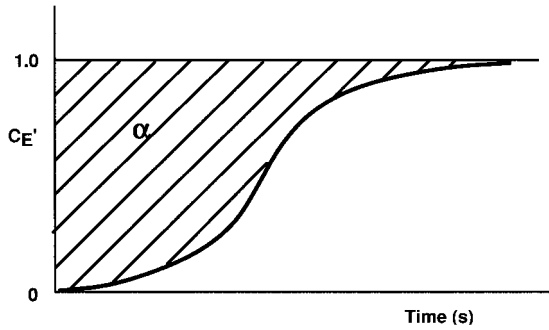


Fig. 3 Determination of the area a above the C_E versus time response curve.

Program

The program KLADYN can be used to investigate the influence of the various experimental parameters on the method, and is formulated in dimensionless form. The same model, but with dimensions, is used in program KLAFIT and is particularly useful for determining $K_L a$ in fitting experimental data of C_E versus time. A set of experimental data in the text file KLADATA can be used to experiment with the data fitting features of MADONNA.

The program ELECTFIT is used to determine the electrode time constant in the first-order lag model. The experiment involves bringing C_E to zero by first purging oxygen from the water with nitrogen and then subjecting the electrode to a step change by plunging it into fully aerated water. The value of the electrode time constant, T_E can be obtained by fitting the model to the set of experimental data in the file ELECTDATA. The value found in this experiment can then be used as a constant in KLAFIT.

Nomenclature

Symbols

C	Oxygen concentration	g/m^3
G	Gas flow rate	m^3/s
H	Henry coefficient	$\text{Pa m}^3/\text{mol}$
$K_L a$	Oxygen transfer coefficient	$1/\text{s}$
RT/H	(Gas constant)(Abs. temp.)/Henry coeff.	–
t	Time	s
V	Reactor volume	m^3
a	Area above C'_E -time (s) curve	s
τ	Time constant	s

Indices

E	Refers to electrode
F	Refers to film
G	Refers to gas phase
L	Refers to liquid
'	Prime denotes dimensionless variables

Exercises

4. Compare the values of the time constants (τ_G , $1/K_L a$, τ_F and τ_E) and the dimensionless groups. For the parameter values used, can you estimate whether all processes will be influential? Check your reasoning by changing the parameters in the simulations and observing the plots of C_G , C_L , C_F and C_E versus time.
5. Verify by simulation that $K_L a$ can be estimated from the value of a , as determined by the area under the curve of Fig. 3.
6. The textbook method for calculating $K_L a$ involves plotting $\ln(1/(1-C'_E))$ versus t to obtain $K_L a$ from the slope. What is the reasoning behind this? For what parameter values would it yield accurate $K_L a$ values? Alter the program to study the characteristics of this plot, investigating its validity for a range of parameters.
7. Vary the time constants for transfer ($1/K_L a$) and for measurement ($\tau_E + \tau_F$) to demonstrate when the measurement response is important.
8. Using the simplification of Exercise 5, estimate the time constants and show how their sum can be estimated from the $C'_G = C'_L = C'_E = 0.63$ position on the curves?
9. Determine T_E using the datafile ELECTDATA together with the program ELECTFIT. Use this value in KLAFIT with the datafile KLADATA to determine $K_L a$ by fitting the model parameter to the data.
10. Instead of using the previously found value of T_E , determine both T_E and $K_L a$ by fitting to the KLADATA file. Compare the fit of the curve and the values of T_E and $K_L a$ found in Exercise 6.

Results

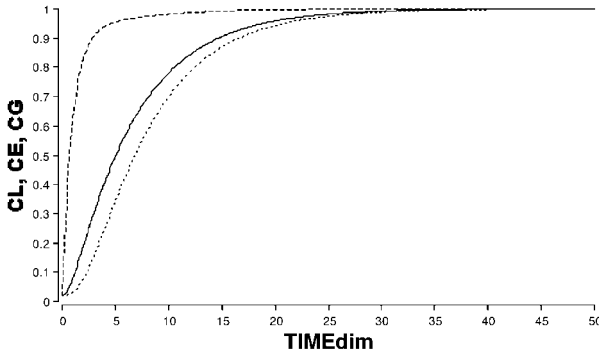


Fig. 4 Response of CG, CL and CE versus TIMEdim from KLADYN.

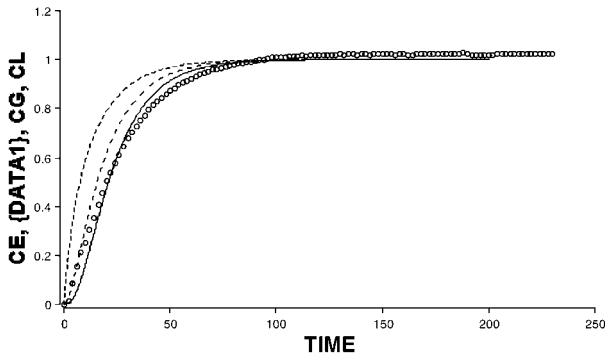


Fig. 5 A fit of experimental data (open circles) as dimensionless CE versus time (s) to determine KLA using KLAFIT, which gives 0.136 1/s. Shown also are CG and CL.

References

- Dang, N.D.P., Karrer, D.A. and Dunn, I.J. (1977) Oxygen Transfer Coefficients by Dynamic Model Moment Analysis, *Biotechnol. Bioeng.* 19, 853.
- Ruchti, G., Dunn, I.J. and Bourne J.R. (1981). Comparison of Dynamic Oxygen Electrode Methods for the Measurement of K_{La} , *Biotechnol. Bioeng.* 13, 277.

5.9.9

AXDISP – Differential Extraction Column with Axial Dispersion**System**

A consideration of axial dispersion is essential in any realistic description of extraction column behaviour. Here a dynamic method of solution is demonstrated, based on a finite differencing of the column height coordinate. Figure 1 below shows the extraction column approximated by N finite-difference elements.

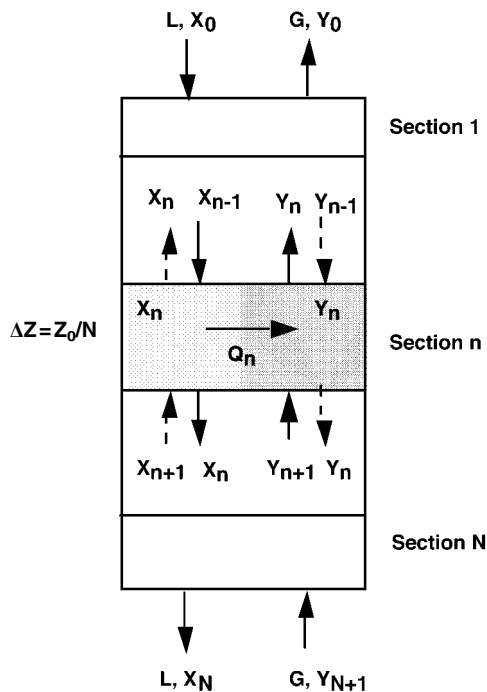


Fig. 1 Axial dispersion model for an extractor.

Model

The detailed derivation of the model equations is described in Sections 4.4.2 and 4.4.3, but are reformulated here in simple concentration terms.

The component balance equations are then:

for the L feed phase

$$\frac{dX_n}{dt} = -E_{1X}(X_{n+1} - X_{n1}) + E_{2X}(X_{n1} - 2X_n + X_{n+1}) - \frac{Q_n}{H_L}$$

and for the G phase

$$\frac{dY_n}{dt} = E_{1Y}(Y_{n+1} - Y_{n-1}) + E_{2Y}(Y_{n-1} - 2Y_n + Y_{n+1}) + \frac{Q_n}{H_G}$$

where the factors E_{1X} and E_{2Y} represent the inverse residence times of the phases, and E_{2X} and E_{2Y} represent the inverse diffusion times of the phases, in segment n .

For the L phase

$$E_{1X} = \frac{L}{A_L \Delta Z} = \frac{v_L}{\Delta Z H_L}$$

$$E_{2X} = \frac{D_L A}{\Delta Z^2 A_L} = \frac{D_L}{\Delta Z^2 H_L}$$

where H_L is the fractional holdup of the L phase. Similar equations apply to the G phase.

The column end sections require special treatment since diffusive flux is obviously absent exterior to the column. Thus, the column outlet concentrations X_{N+1} and Y_0 are based on an extrapolation of the concentration profiles over the additional half outlet section of the column, as again described in Sections 4.4.2 and 4.4.3.

Thus for the L and G phase flows leaving end section 8

$$\frac{dX_N}{dt} = E_{1X}(X_{N-1} + X_N - 2X_{N+1}) + E_{2X}(X_{N-1} - X_N) - \frac{Q_N}{H_L}$$

$$\frac{dY_N}{dt} = E_{1Y}(2Y_{N+1} - (Y_{N-1} + Y_N)) + E_{2Y}(Y_{N-1} - Y_N) + \frac{Q_N}{H_G}$$

The balances for the other end section, $n=1$, take a similar form.

Program

The simulation starts with the initial axial concentration profiles set to zero. Using arrays, the number of sections is set by the parameter N_{slabs} , allowing the axial concentration profile for each phase along the contactor to be demonstrated.

Nomenclature

Symbols

D	Eddy dispersion coefficient	cm^2/s
E_1	Inverse residence time	$1/\text{s}$
E_2	Inverse dispersion time	$1/\text{s}$

H	Fractional phase holdup	–
L and G	Superficial phase velocity	cm/s
Q	Mass transfer rate	$\text{g/cm}^3 \text{ s}$
X and Y	Solute concentration	g/cm^3
Z	Column height	cm

Indices

*	Equilibrium value
n	Stage n
L and G	Liquid phase

Exercises

1. The steady-state outlet values should be checked for the overall balance.
2. The extent of extraction can be investigated as a function of solvent flow rate.
3. The mass transfer coefficient can be increased to obtain an approach to equilibrium conditions.
4. The dispersion coefficients can be increased to observe an approach to ideal mixing. Setting the coefficients to zero should give the best performance.
5. The dynamic responses for changes in inlet conditions can be investigated.

Results

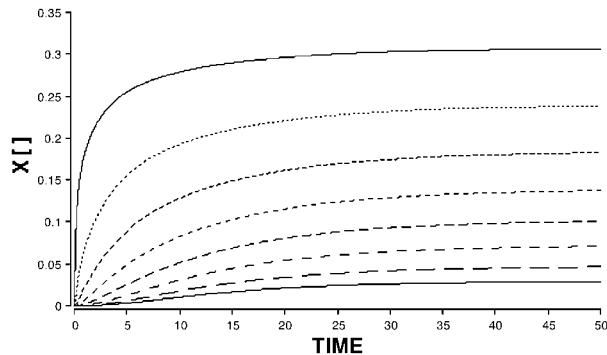


Fig. 2 Time-dependent concentration variations for the L-phase [$D_L = D_G = 100$].

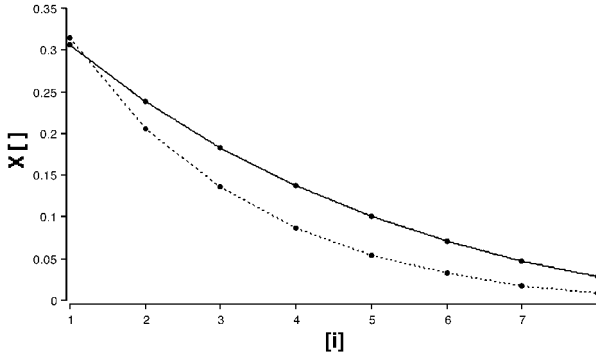


Fig. 3 Steady state concentration profiles for the L-phase [$D_L = D_G = 100$] and [$D_L = D_G = 20$].

5.9.10

AMMONAB – Steady-State Design of a Gas Absorption Column with Heat Effects

System

Ammonia is recovered from an air–ammonia gas mixture by absorption into water, using a countercurrent packed column. The absorption is accompanied by the evolution of heat which causes a rise in the water temperature and hence a change in the equilibrium. The problem and data values are taken from Backhurst and Harker (1990).

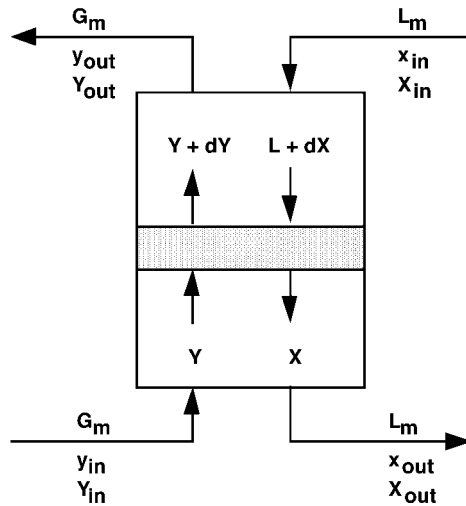


Fig. 1 Steady-state ammonia absorption column.

Model

The gas is at high concentration and therefore the column component balance equations are based on mole ratio concentration units.

The balance equations for countercurrent flow follow Section 4.4.1.

For the gas

$$\frac{dY}{dz} = \frac{K_G a (y - y_e)}{L_m}$$

For the liquid

$$\frac{dX}{dz} = \frac{K_G a (y - y_e)}{G_m}$$

The liquid phase energy balance is given by

$$\frac{dT}{dz} = \frac{K_G a (y - y_e) \Delta H}{L c_p}$$

The temperature in the gas phase is assumed constant with no heat losses and zero gas-liquid heat interchange.

The equilibrium relationship is represented by

$$y_e = \frac{KX}{P_T}$$

where the equilibrium constant, K , is a function of temperature.

The inlet gas flow is $1.25 \text{ m}^3/\text{m}^2 \text{ s}$ measured at NTP containing 5% by volume NH_3 . Hence

$$G_m = (1.25)(0.95)/22.4 = 0.053 \text{ kmol}/\text{m}^2 \text{ s}$$

For Y_{in} equal 0.05

$$Y_{\text{in}} = 0.05/0.95 = 0.0526 \text{ kmol NH}_3/\text{kmol air}$$

For 95% ammonia recovery

$$Y_{\text{out}} = \frac{0.0526 * 0.05}{1 + 0.0526 * 0.05} = 0.00263 \text{ kmol NH}_3/\text{kmol air}$$

The inlet water flow is $1.95 \text{ kg}/\text{m}^2 \text{ s}$, hence

$$L_m = 195/18 = 0.108 \text{ kmol}/\text{m}^2 \text{ s}$$

An overall component balance for the column gives

$$G_m(Y_{in} - Y_{out}) = L_m(X_{out} - X_{in})$$

Calculating the concentration in the outlet liquid

$$X_{out} = \frac{0.053 * (0.0526 - 0.00263)}{0.108} = 0.0245 \text{ kmol NH}_3/\text{kmol water}$$

Backhurst and Harker present the equilibrium data as straight line relationships for the temperatures 293 K, 298 K and 303 K. This data was curve fitted to the form

$$y_e = \frac{Kx}{P_T}$$

where $K = a + bT + cT^2$, and the constants are given by $a = 0.0059$, $b = 0.1227$ and $c = 3.01$.

Program

The program starts from the known concentration and temperature conditions at the top of the column and integrates down the column until the condition Y_{in} (calculated) is equal to the known inlet value Y_{in} . A variable Y_{height} is defined in the program to locate the Y_{IN} position. Note the use of HEIGHT, instead of TIME, as the independent variable in this steady state example.

Nomenclature

Symbols

c_p	Specific heat	$\text{kJ/kmol } ^\circ\text{C}$
G_m	Molar flow of inert air	$\text{kmol/m}^2 \text{ s}$
K	Equilibrium constant	kN/m^2
K_{Ga}	Overall mass transfer capacity coefficient based on the gas phase Δy	$\text{kmol/m}^3 \text{ s}$
L_m	Molar flow of solute-free water	$\text{kmol/m}^2 \text{ s}$
P_T	Pressure	kN/m^2
ρ	Density	kg/m^3
T	Liquid temperature	$^\circ\text{C}$
X	Mole ratio concentration in the liquid phase	–
x	Mole fraction concentration in the liquid phase	–
Y	Mole ratio concentration in the gas phase	–
y	Mole fraction concentration in the gas phase	–
z	Height of packing	m
ΔH	Exothermic heat of adsorption	kJ/kmol

Indices

in, out Refer to inlet and outlet conditions
e Refers to equilibrium

Exercises

1. Study the effects of varying liquid rate, inlet water temperature, inlet gas concentration and pressure on the absorption.
3. Modify the program so that you are able to graph the driving force for mass transfer ($y - y_e$) and the resulting “pseudo” equilibrium curve, i.e., (y_e versus x), allowing for the changing temperature. Note however that the equilibrium relationship is only valid for the range 293 to 303 K.
3. Develop a dynamic model for the column and compare its flexibility with this steady state model.

Results

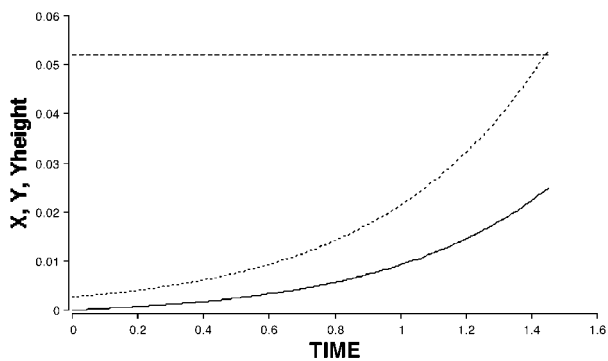


Fig. 2 Gas and liquid concentrations where the required column height is determined as 1.45 m.

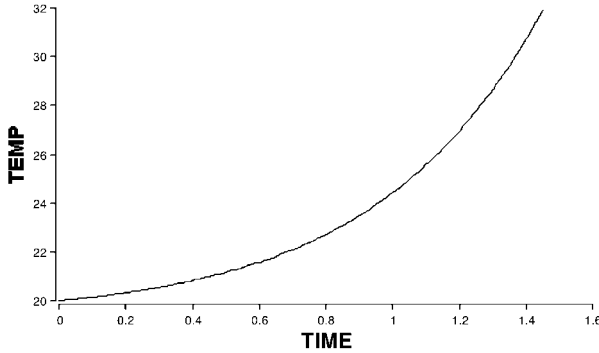


Fig. 3 The corresponding variation in the liquid phase temperature for the column of column height of 1.45 m, as determined in Fig. 2.

Reference

Backhurst, J.R. and Harker, J.H. (1990) Chemical Engineering, Vol. 5, Pergamon.

5.9.11

MEMSEP – Gas Separation by Membrane Permeation

System

An internally staged gas-permeation module is used for the oxygen enrichment of air, using the flow arrangement shown in Fig. 1. Enrichment depends on differing membrane permeabilities for the oxygen and nitrogen to be separated. The permeation rates are proportional to the differences in component partial pressures.

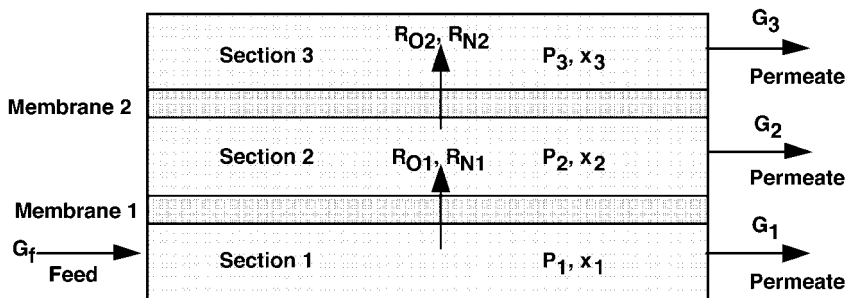


Fig. 1 Configuration of the gas-permeation module.

Model

The module system consists of three well mixed sections, separated by two membranes. Overall steady-state balances can be used to check the computer solution and are given by

Total mass:

$$N_f = N_1 + N_2 + N_3$$

Oxygen:

$$N_f x_{OF} = N_1 x_{O1} + N_2 x_{O2} + N_3 x_{O3}$$

Nitrogen:

$$N_f(1 - x_{OF}) = N_1(1 - x_{O1}) + N_2(1 - x_{O2}) + N_3(1 - x_{O3})$$

Steady-state total mass balances can also be written for Sections 1, 2 and 3, based on the flow rates in each section and the permeation rates between sections. Converting from mol/s to m³/s using the Ideal Gas Law gives

Section 1

$$G_f = G_1 + (R_{O1} + R_{N1}) \frac{RT}{P_1}$$

Section 2

$$G_2 = (R_{O2} + R_{N2} - R_{O1} - R_{N1}) \frac{RT}{P_2}$$

Section 3

$$G_3 = (R_{O2} + R_{N2}) \frac{RT}{P_2}$$

The dynamic component mass balances in terms of concentrations are as follows:

Section 1

$$\text{Oxygen} \quad \frac{dC_{O1}}{dt} = \frac{G_f C_{Of} - G_1 C_{O1} - R_{O1}}{V_1}$$

$$\text{Nitrogen} \quad \frac{dC_{N1}}{dt} = \frac{G_f C_{Nf} - G_1 C_{N1} - R_{N1}}{V_1}$$

Section 2

$$\text{Oxygen} \quad \frac{dC_{O_2}}{dt} = \frac{R_{O_1} - G_2 C_{O_2} - R_{O_2}}{V_2}$$

$$\text{Nitrogen} \quad \frac{dC_{N_2}}{dt} = \frac{R_{N_1} - G_2 C_{N_2} - R_{N_2}}{V_2}$$

Section 3

$$\text{Oxygen} \quad \frac{dC_{O_3}}{dt} = \frac{R_{O_2} - G_3 C_{O_3}}{V_3}$$

$$\text{Nitrogen} \quad \frac{dC_{N_3}}{dt} = \frac{R_{N_2} - G_3 C_{N_3}}{V_3}$$

The permeation rate is proportional to the partial pressure difference, the membrane permeability, its area and thickness:

Section 1 to Section 2:

$$\text{For } O_2 \quad R_{O_1} = \frac{k_{pO}}{d} (P_1 x_{O_1} - P_2 x_{O_2}) A_1$$

$$\text{For } N_2 \quad R_{N_1} = \frac{k_{pN}}{d} (P_1 (1 - x_{O_1}) - P_2 (1 - x_{O_2})) A_1$$

Section 2 to Section 3:

$$\text{For } O_2 \quad R_{O_2} = \frac{k_{pO}}{d} (P_2 x_{O_2} - P_3 x_{O_3}) A_2$$

$$\text{For } N_2 \quad R_{N_2} = \frac{k_{pN}}{d} (P_2 (1 - x_{O_2}) - P_3 (1 - x_{O_3})) A_2$$

Program

The program employs an IF THEN ELSE statement to switch the feed rates. An alternative with the Windows version of MADONNA would be to use the CONTINUE feature. For this, the values of N_f would be changed after the STOPTIME was reached and the run continued with a new value of N_f and STOPTIME.

Nomenclature**Symbols**

A	Membrane area	m^2
C	Concentration	mol/m^3
d	Membrane thickness	m
G	Flow rate	m^3/s
K_C	Cost constant	$1/Pa^2$
k_p	Permeability coefficient	$mol/m \text{ s Pa}$
N	Molar flow rate	mol/s
P	Pressure	Pa
R	Gas constant	$m^3 \text{ Pa/mol K}$
R_{in}	Permeation rate	mol/s
V	Section volume	m^3
x	Mole fraction of oxygen	–

Indices

1, 2, 3	Sections 1, 2, 3 and membrane 1, 2
O	Oxygen
N	Nitrogen
f	Feed

Exercises

1. Study the influence of pressures P_1 and P_3 on the separation performance.
2. Introduce new membranes with improved permeabilities to give better separation and test them by simulation.
3. Define a cost function assuming that the cost increases with P_1^2 and G_f and that the enrichment of stream 3 gives profits according to

$$COST = P_1^2 G_f - K_C x_{O_3} G_3$$

Use a reasonable value for K_C and then try to find the optimum by varying the pressure in the three stages.

Results

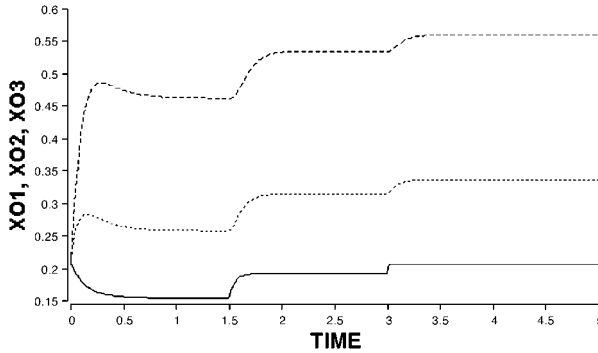


Fig. 2 Mole fractions in the three stages at varying feed flow rate ($G_f=0.05, 0.2$ and $2 \text{ m}^3/\text{s}$).

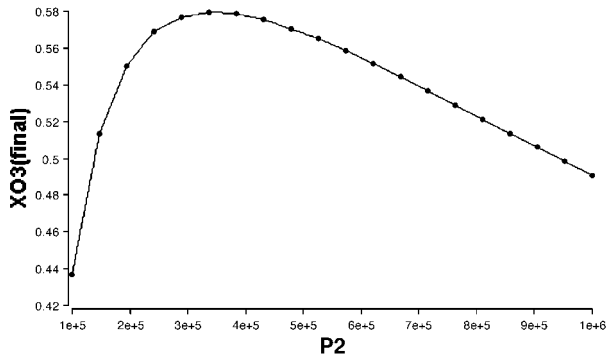


Fig. 3 Influence of P_2 on oxygen mole fractions in the third stage, $N_f=50 \text{ mol/s}$ (range of $P_2=0.1$ to $1.0 \cdot 10^6 \text{ Pa}$).

Reference

Li, K., Acharya, R. and Hughes, R. (1991) Simulation of Gas Separation in an Internally Staged Permeator, *Trans. IChemE.* 69, Part A, 35–42.

5.9.12

FILTWASH – Filter Washing

System

The washing of filter cake is carried out to remove liquid impurities from the valuable solid filter cake or to increase the recovery of valuable filtrate. Wake-man (1990) has shown that the axial dispersion flow model, as developed in

Section 4.3.6, provides a fundamental description of cake washing and can take into account the influence of many phenomena. These include non-uniformities in the liquid flow pattern, non-uniform porosity distributions, the initial spread of washing liquid onto the topmost surface of the filter cake and the desorption of solute from the solid surfaces.

Model

As shown by Wakeman, the solute material balance for the flowing liquid phase, allowing for axial dispersion and desorption of solute is given by the following defining partial differential equation

$$\frac{\partial c}{\partial t} + \frac{(1 - \varepsilon)}{\varepsilon} \frac{\partial \eta}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x}$$

The concentration of the solute adsorbed on to the particles is related to the concentration of the solute in the liquid by an equilibrium relationship of the form

$$\eta = K_0 + Kc^{1/N}$$

Expressing the model equations in dimensionless form gives

$$\frac{\partial c'}{\partial W} \left[1 + \frac{Kc'^{(1-N)/N}}{N} \left(\frac{1 - \varepsilon}{\varepsilon} \right) c'^{(1-N)/N} \right] = P \frac{\partial^2 c'}{\partial x'^2} - \frac{\partial c'}{\partial x'}$$

where

$$c' = \frac{c}{c_0} \quad \text{and} \quad x' = \frac{x}{L}$$

W is the wash ratio given by

$$W = \frac{u_{x=0}t}{L}$$

and P is the Peclet number

$$P = \frac{D_L}{u_{x=0}L}$$

For solution by digital simulation the depth of the filter cake is finite differenced, each element having a dimensionless thickness Δx . For any element n the resulting difference differential equation is given by

$$\frac{dc_n}{dW} = \frac{1}{Z} \left[P \frac{c_{n-1} - 2c_n + c_{n+1}}{\Delta x^2} - \frac{c_{n+1} - c_{n-1}}{2\Delta x} \right]$$

where the term Z is given by

$$Z = 1 + \frac{Kc_0^{(1-N)/N}}{N} \frac{1 - \varepsilon}{\varepsilon} c_i^{(1-N)/N}$$

In these equations the prime designation for dimensionless concentration, c' , has been dropped.

Program

Program **FILTWASH** models the dimensionless filtration wash curves for the above case of a filter cake with constant porosity, axial dispersion in the liquid flow and desorption of solute from the solid particles of the filter bed.

Limit values on concentration are very important in the program, in order to avoid possible numerical overflow problems, caused by zero concentration values in the denominator of the model equations.

Special relationships apply to the end segments, owing to the absence of axial dispersion exterior to the cake.

Nomenclature

Symbols

c	Solute concentration in liquid	kg/m^3
c'	Dimensionless solute concentration	—
c_0	Solute conc. in cake before washing	kg/m^3
D_L	Axial dispersion coefficient	m^2/s
K_0	Constant in equilibrium isotherm	kg/m^3
K	Adsorption equilibrium constant	$\left(\frac{\text{kg m}^3}{\text{m}^3 \text{ kg}}\right)^{-1/N}$
L	Cake thickness	m
N	Reciprocal order of the adsorption	—
P	Peclet number per unit volume of voids	—
S	Fractional saturation, volume of liquid	—
t	Time	s
u	Pore velocity	m/s
W	Wash ratio	—
x	Distance measured from filter cloth	m
x^*	Dimensionless distance	—
ε	Cake porosity	—
η	Solute concentration on solid	kg/m^3

Exercises

1. Use the program to assess the effects of differing degrees of axial dispersion, for values of Peclet number ranging from 0.005 to 0.25. Modify the program to account for zero axial dispersion.
2. Wakeman found that the effect of increasing the equilibrium constant in the description isotherm equation is to increase the wash-ratio required. Is this confirmed by simulation, and what is the explanation of this effect?
3. Increasing the value of N (reciprocal power term) reduces the effect of the desorbed solute and agrees ultimately with the case of zero solute desorption. Try this in a parametric run.
4. In compressible filter cakes, the porosity varies from a minimum next to the filter septum to a maximum at the cake surface. How could you include such a variation within the context of a simulation program? Remember that as the porosity changes, the local fluid velocity will also change as a result of

$$(u\varepsilon)_{x'} = (u_{x'=0})(\varepsilon_{x'=0})$$

A necessary assumption would also be that the initial porosity distribution remains constant and independent of flow rate.

5. The presence of a liquid layer on the surface of the filter cake will cause solute to diffuse from the top layer of cake into the liquid. Also if disturbed, the layer of liquid will mix with the surface layer of filter cake. This effect can be incorporated into a simulation by assuming a given initial depth of liquid as an additional segment of the bed which mixes at time $t=0$ with the top cake segment. The initial concentrations in the liquid layer and in the top cake segment are then found by an initial mass balance. Try altering the model to account for this.

Cases 4 and 5 are solved also by Wakeman (1990).

Results

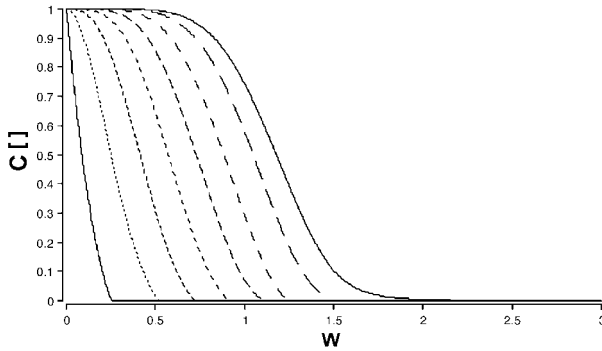


Fig. 1 Solute concentration variations as a function of wash ratio.

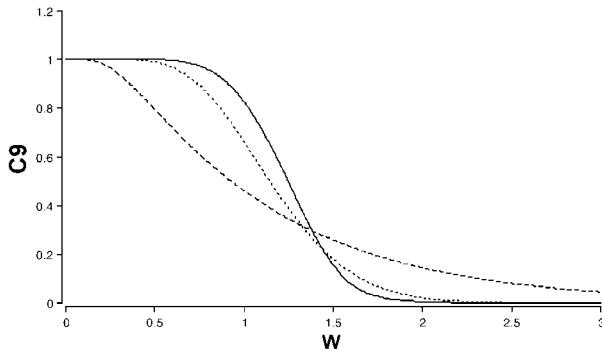


Fig. 2 Variations in outlet solute concentrations [$D_L=8.5E-8$], [$D_L=8.5E-7$] and [$D_L=8.5E-6$].

References

- Wakeman, R.J. (1990) *Chem. Eng. Res. Des.* 68, 161–171.
 Wakeman, R.J. (1986) *Chem. Eng. Res. Des.* 64, 308.
 Wakeman, R.J. (1981) in “Solid–Liquid Separation”, ed. L. Svarovsky, Butterworths, London.

5.9.13

CHROMDIFF – Dispersion Rate Model for Chromatography Columns

System

As explained in Section 4.4.4, the movement of components through a chromatography column can be modelled by a two-phase rate model, which is able to handle multicomponents with nonlinear equilibria. In Fig. 1 the column with seg-

ment n is shown and in Fig. 2 the structure of the model is depicted. This involves the writing of separate liquid and solid phase component balance equations, for each segment n of the column. The movement of the solute components through the column occurs by both convective flow and axial dispersion within the liquid phase and by solute mass transfer from the liquid phase to the solid.

Model

The equations have previously been derived in Section 4.4.4 in a form suitable for programming with MADONNA. Correlations for the column Peclet number are taken from the literature and used to calculate a suitable value for the dispersion coefficient for use in the model.

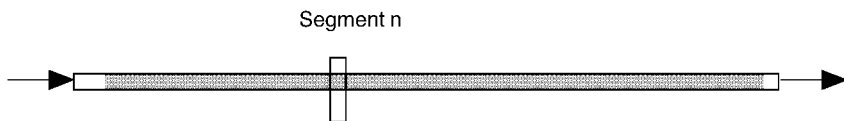


Fig. 1 Chromatographic column showing finite differencing into column segments.

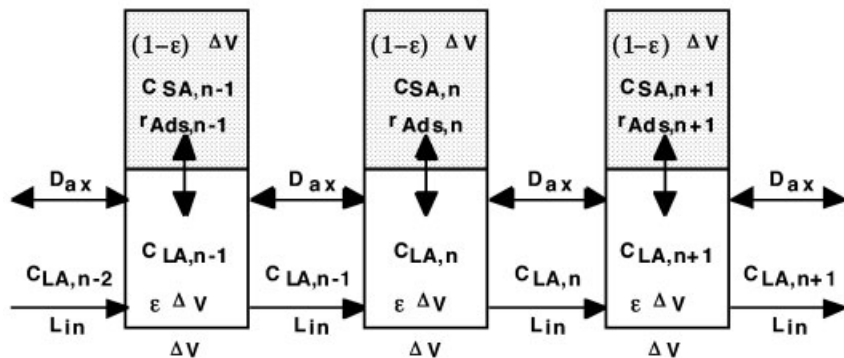


Fig. 2 Structure of the two-phase rate model in finite-difference form.

Program

The model is written in vector form with the last elements taken separately to satisfy the closed end boundary conditions.

Nomenclature

Refer to the nomenclature in Section 4.4.4 and in the program.

Exercises

1. Study the influence of the equilibrium constant ratio K_B/K_A , for the two components A and B, on the resolution of the peaks, as given by the time difference between the peaks.
2. The liquid flow rate directly influences the dispersion coefficient. Investigate its influence on peak width.
3. Correlate the degree of separation obtained as a function of column Peclet number and compare this to the number of theoretical plates required in simulation example CHROMPLATE for a similar degree of separation obtained.
4. Investigate the influence of increasing column length on the degree of separation obtained, by varying the increment number NN, but with constant ΔZ . Keeping NN constant, now vary the length of column by increasing the length of each increment.
5. Amend the program to allow for interacting non-linear Langmuir equilibria for the two components, as given below, using the following numerical equilibrium values $K_A=3$, $K_B=1.8$, $b_A=2$ and $b_B=4$.

$$C_{SA}^* = \frac{K_A C_{LA}}{1 + b_A C_{LA} + b_B C_{LB}} \quad C_{SB}^* = \frac{K_B C_{LB}}{1 + b_A C_{LA} + b_B C_{LB}}$$

Results

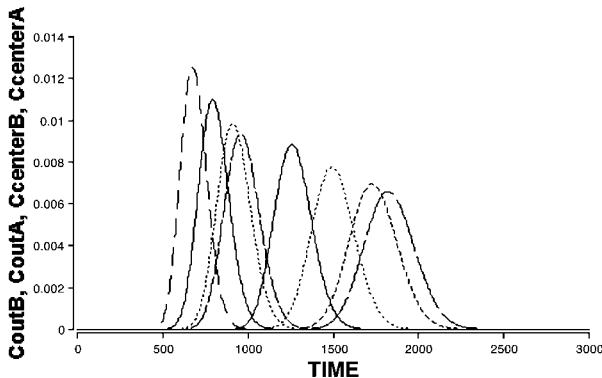


Fig. 3 Decrease of resolution caused by increasing K_B (1.8, 2.3 and 2.8) in 3 runs.

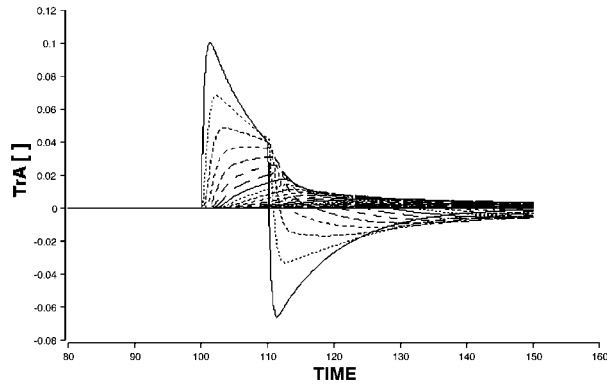


Fig. 4 Transfer rate at the time of the pulse injection, showing direction reversal.

Reference

Strube, J. (1999) Plant Engineering and Design Course Notes, University of Dortmund.

5.9.14

CHROMPLATE – Stagewise Linear Model for Chromatography Columns

System

As explained in Section 4.4.4, there exists an equivalency between tubular dispersion models and stagewise or tank in series models. The stagewise model, used in CHROMPLATE considers the chromatographic column to consist of a large number of well-mixed stirred tanks, arranged in series and thus represents an alternative modelling approach to that of the tubular dispersion model CHROMDIFF. The same two-component separation process is modelled and simulated in both cases.

Each tank contains a known quantity of both solid adsorbant and liquid phase. As depicted in Figs. 1 and 2, only the liquid phase is mobile and the solid phase remains static. Both phases contain solute components A and B, which move along the column, from stage to stage, only by convective flow.

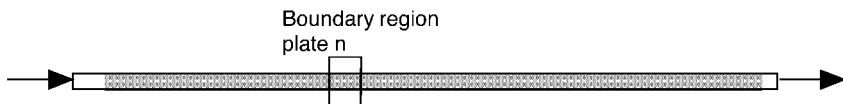


Fig. 1 Chromatographic column showing a mass balance region.

Taking a balance for component A around both phases in stage n gives

$$\left(\begin{array}{c} \text{Accumulation} \\ \text{in the} \\ \text{liquid phase} \end{array} \right) + \left(\begin{array}{c} \text{Accumulation} \\ \text{in the} \\ \text{solid phase} \end{array} \right) = \left(\begin{array}{c} \text{Flow} \\ \text{in} \end{array} \right) - \left(\begin{array}{c} \text{Flow} \\ \text{out} \end{array} \right)$$

$$\varepsilon V_{\text{stage}} \frac{d(C_{LA,n})}{dt} + (1 - \varepsilon) V_{\text{stage}} \frac{d(C_{SA,n})}{dt} = L_{\text{in}}(C_{LA,n-1} - C_{LA,n})$$

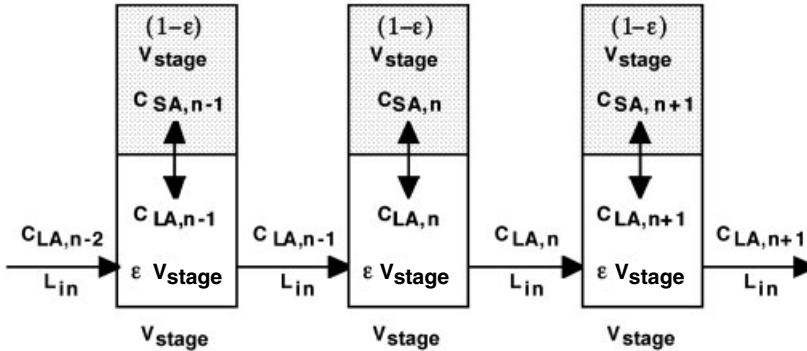


Fig. 2 Plate model with equilibrium stages.

Taking the balance, around both phases, effectively disregards the rate of solute transfer from liquid to solid and, instead, the assumption of a perfect equilibrium stage is employed to provide a relation between the resulting liquid and solid phase concentrations. For the special case of a linear equilibrium

$$C_{LA} = K_A C_{SA}$$

Practical adsorption isotherms are usually more complex, especially at high concentrations. But for the linear equilibrium employed here, the analysis becomes very simple. Combining the equilibrium relationship with the balance equation yields

$$\frac{d(C_{LA,n})}{dt} = \frac{L_{\text{in}}(C_{LA,n-1} - C_{LA,n})}{\varepsilon V_{\text{stage}} + (1 - \varepsilon) V_{\text{stage}} K_A}$$

A similar balance equation can be written for the second component B. Thus the resulting model consists of $2 \cdot N$ equations, where N is the number of stages in the cascade. These are then easily solved by simulation.

It should be noted that taking the balance region over both the combined phases, as done in this example, is useful only for linear equilibrium. In general the best method is to use a transfer rate model, as described in Section 4.4.4, and to make balances for each component in each phase separately.

Nomenclature**Symbols**

V_{stage}	Volume of a single plate section	cm^3
C_L	Liquid phase concentration	g/cm^3
C_S	Solid phase concentration	g/cm^3
d	Tube diameter	cm
D_p	Diameter of packing particle	cm
ε	Fraction voids	–
k and k_{eff}	Mass transfer rate coefficient	$1/\text{s}$
K	Equilibrium constant	–
L_{in}	Volumetric flow rate	cm^3/s
L_{bed}	Length of column	cm

Subscripts

A	Refers to component
B	Refers to component
in	Refers to inlet
L	Refers to liquid phase
n	Refers to stage number
S	Refers to solid phase adsorbent

Exercises

1. Study the effect of differing number of stages.
2. Investigate the influence of flow rate on the separation.
3. Vary the equilibrium constants to quantify their influence.
4. Choose values of the equilibrium constant so that the separation is difficult. Run simulations with increased column length or number of plates to improve the separation.
5. Write a program for this stagewise model using transfer rates as in CHROM-DIFF.

Results

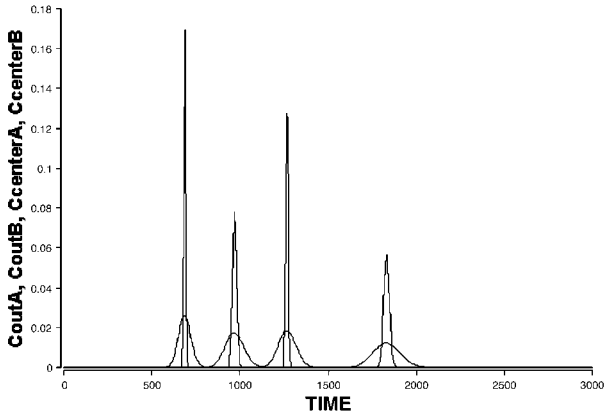


Fig. 3 Separation of A and B for 500 and 5000 plates at center and end of column.

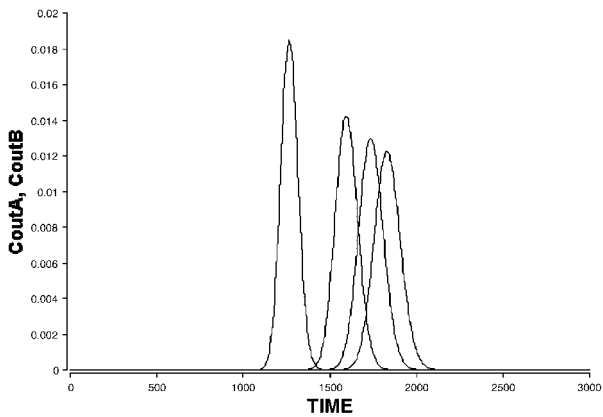


Fig. 4 As K_B is increased (1.8, 2.5 and 2.8) the B peak moves toward the A peak.

Reference

Strube, J. (1999) Plant Engineering and Design Course Notes, University of Dortmund.