

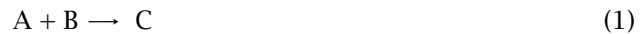
Process Systems Steady-State Modeling and Design

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1 Process Flow Diagram

Our goal is to develop a process for the production of chemical C from raw materials A and B. Reaction 1 is carried out in reactor RC.



Due to thermodynamic limitations (that we will study in CBE 311), the conversion of A and B into C is not complete; it reaches equilibrium, a state where raw materials A and B, and product C coexist at a specific ratio K_{eq} . Hence, the effluent of the reactor (stream S_3) is fed into flash tank FT to separate the heavy C from the more volatile A and B. Product C is removed in the liquid stream S_5 , whereas a fraction R of the vapor stream S_4 is recycled

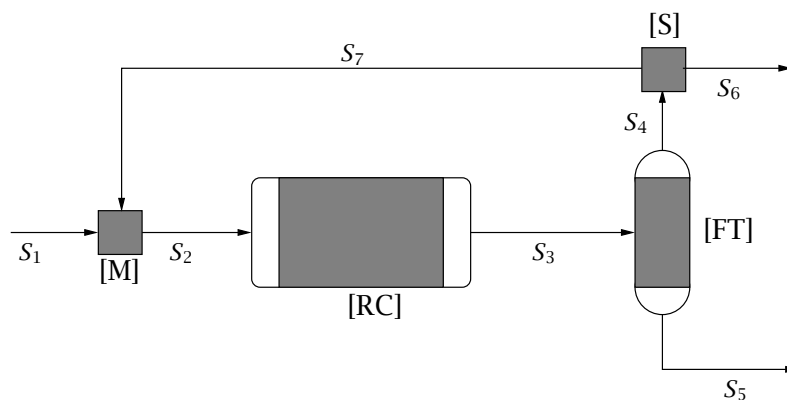


Figure 1: Process flow diagram for the production of C from A and B.

back to the process (stream S_7). The input stream S_2 of the reactor is obtained by mixing streams S_7 and S_1 . A diagram of the process is shown in Figure 1.

2 Material Balances

To rigorously study this system, we need to have a tool that allows us to calculate the molar flows of the three chemicals in the seven process streams. In other words, we need to develop a model that describes this system. This model is based on the material balance equations for the three components. If N_j^k is the molar flow (kmol/hr) of chemical $j \in \{A, B, C\}$ in stream $k \in \{S_1, S_2, S_3, S_4, S_5, S_6, S_7\}$, then we can express the following equations.

Mixer (M). Streams S_1 and S_7 are mixed to give stream S_2

$$N_j^{S_2} = N_j^{S_1} + N_j^{S_7} \quad j \in \{A, B, C\} \quad (2)$$

Reactor (RC). If ξ is the extent of the reaction (i.e. the production of C in kmol/hr), then the molar flows in the effluent stream S_3 are given by the following equations

$$N_j^{S_3} = N_j^{S_2} + \xi v_j \quad j \in \{A, B, C\} \quad (3)$$

in which v_j is the stoichiometric coefficient of component j in Reaction 1; i.e. $v_A = -1$, $v_B = -1$, and $v_C = 1$. If Q^{S_3} is the volumetric flow (m^3/hr) of stream S_3 , then equilibrium is described by

$$\begin{aligned} K_{\text{eq}} &= \frac{c_C^{S_3}}{c_A^{S_3} c_B^{S_3}} = \frac{N_C^{S_3} / Q^{S_3}}{(N_A^{S_3} / Q^{S_3})(N_B^{S_3} / Q^{S_3})} \\ K_{\text{eq}} &= Q^{S_3} \frac{N_C^{S_3}}{N_A^{S_3} N_B^{S_3}} \end{aligned} \quad (4)$$

If we assume an ideal mixture (another topic covered in CBE 311) and that the densities of A, B and C are practically the same and equal to ρ , then the volumetric flow of S_3 can be calculated by

$$Q^{S_3} = \frac{M_A N_A^{S_3} + M_B N_B^{S_3} + M_C N_C^{S_3}}{\rho} \quad (5)$$

in which M_j is the molar weight of component j . Exercise 8 considers the case in which the mixture density is not constant.

Flash tank (FT). Flash tanks are designed to carry out specified separation tasks. In this case, our goal is to recover C in the liquid stream S_5 and the two (volatile) raw materials, A and B, in the vapor stream S_4 . If ϕ_j is the fraction of the flow of chemical j that is

recovered in the vapor stream (split fraction), then the molar flows in streams S_4 and S_5 can be calculated as follows:

$$N_j^{S_4} = \phi_j N_j^{S_3} \quad j \in A, B, C \quad (6)$$

$$N_j^{S_5} = (1 - \phi_j) N_j^{S_3} \quad j \in A, B, C \quad (7)$$

Splitter (S). A fraction R of stream S_4 is recycled back to the process (stream S_7), while the remaining stream is purged (stream S_6). Note that the relative amounts of compounds A, B and C in streams S_6 and S_7 are identical and equal to the relative amounts in stream S_4 . Hence, the molar flows in S_6 and S_7 are:

$$N_j^{S_6} = (1 - R) N_j^{S_4} \quad j \in A, B, C \quad (8)$$

$$N_j^{S_7} = R N_j^{S_4} \quad j \in A, B, C \quad (9)$$

Equations 2-9 fully describe the process in Figure 1. But how can we solve these equations, i.e. find values of variables that simultaneously satisfy them?

3 Newton's Method

In this section, we will study how we can find the root of a nonlinear equation $f(x) = 0$, i.e. find the value of x at which function f becomes zero. We consider equation:

$$f(x) = x^3 - 2x^2 + 3x - 6 = 0 \quad (10)$$

Let $x^0 = 1$ be our initial guess. The value of f at $x^0 = 1$ is $f(1) = -4 \neq 0$. Our initial guess was incorrect. To make a new guess, we have to first determine whether the root is larger or smaller than 1. We check the derivative of f at $x = 1$: $f'(x) = 3x - 4x + 3$ which gives $f'(1) = 2$. Since $f(1) = -4$ and f increases at $x = 1$, the root must be larger than 1. But how much larger? If we assume that f increases at a rate equal to $f'(1)$ (and for now this is a reasonable assumption), then the root x^* should be given by:

$$x^* = x^0 - \frac{f(x^0)}{f'(x^0)} \quad (11)$$

which is derived from the definition of the slope between points $(x^0, f(x^0))$ and $(x^*, f(x^*))$

$$f'(x^0) = \frac{f(x^*) - f(x^0)}{x^* - x^0}$$

with $f(x^*) = 0$, because x^* is supposed to be the root of f . Unfortunately, nonlinear functions do not increase at a constant rate. Thus, the x^* calculated in Equation 11 is not going to be the root of f (check: $x^* = 3$ and $f(x^* = 3) = 12$). However, not everything is lost: the new x calculated in Equation 11 can be our next estimate x^1 . This is the main

Iteration k	x^k	$f(x^k)$	$f'(x^k)$
0	1.0000	-4.0000	2.0000
1	3.0000	12.0000	18.0000
2	2.3333	2.8148	10.0000

Table 1: Iterations of Newton's method.

idea behind Newton's method, an iterative scheme for the solution of nonlinear equations: given a point (estimate) x^k at the current iteration k , we calculate our next point using:

$$x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)} \quad (12)$$

The ratio $-f(x^k)/f'(x^k)$ in the right-hand side of this equation is the step we have to take to move towards the root. The numerator tells us how big the gap is, and the denominator tells us how fast we can close this gap. The step $p^k = -f(x^k)/f'(x^k)$ is called the Newton step. In the Newton's algorithm we take successive steps until $f(x^k)$ becomes (almost) zero. The steps of the Newton's algorithm are as follows:

0. Set $k = 0$; choose tolerance ϵ ; guess x^0 .
1. Calculate step $p^{k+1} = -f(x^k)/f'(x^k)$; new estimate $x^{k+1} = x^k + p^{k+1}$.
2. If $f(x^{k+1}) < \epsilon$ stop: x^{k+1} is a root of $f(x) = 0$; otherwise, set $k = k + 1$ and go to 1.

The first two iterations of Newton's method for Equation 10 are shown in Figure 2 and Table 1.

4 Solution of Systems of Nonlinear Equations

In many engineering applications we have to solve systems of nonlinear equations. Such applications include nonlinear least squares, numerical solution of ordinary differential equations, and steady state calculations of chemical processes as the one we examined in Sections 1 and 2. A system of nonlinear equations in n unknowns can be written as follows

$$\begin{aligned} f_1(x_1, x_2, \dots, x_n) &= 0 \\ f_2(x_1, x_2, \dots, x_n) &= 0 \\ &\dots \\ f_n(x_1, x_2, \dots, x_n) &= 0 \end{aligned}$$

or using vector notation

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

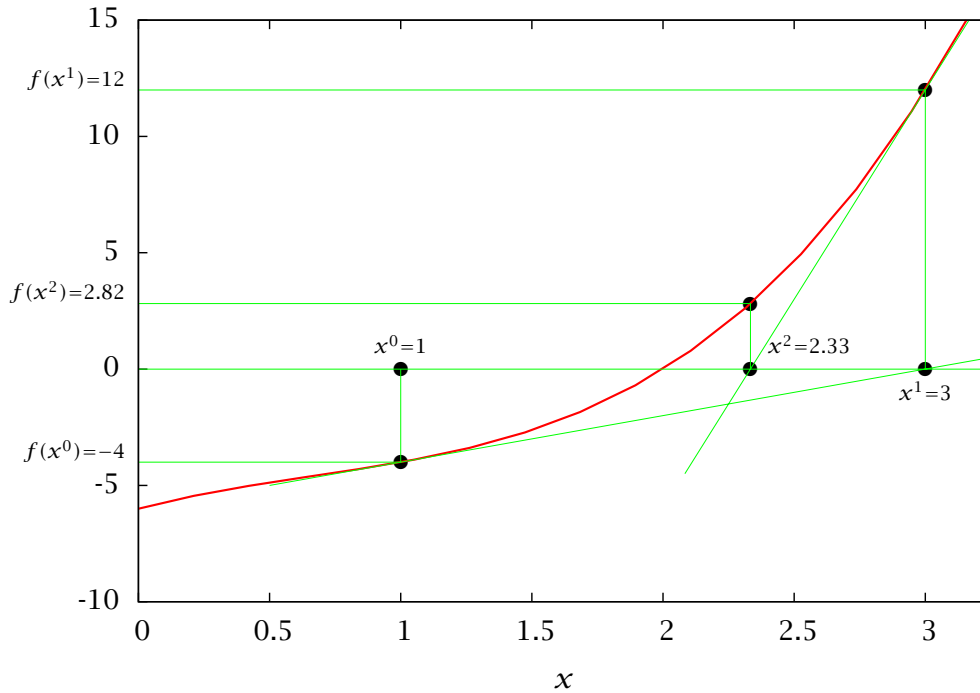


Figure 2: Two iterations of Newton's method for $f(x) = x^3 - 2x^2 + 3x - 6 = 0$.

in which $\mathbf{f} = [f_1 \ f_2 \ \dots \ f_n]^T$ is a vector of nonlinear functions in n variables (x_1, x_2, \dots, x_n) . To solve a system of equations, we can generalize the idea of Newton's method: given an estimate $\mathbf{x}^k = [x_1^k \ x_2^k \ \dots \ x_n^k]^T$ at the current iteration k , we want to find a new estimate \mathbf{x}^{k+1} that is closer to the solution \mathbf{x}^* . In this case, the change of multivariable function \mathbf{f} will depend on the partial derivatives of \mathbf{f} with respect to variables (x_1, x_2, \dots, x_n) . Thus, the general formula for the Newton step for systems of equations is:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{J}(\mathbf{x}^k)^{-1} \mathbf{f}(\mathbf{x}^k) \quad (13)$$

in which $\mathbf{J}(\mathbf{x}^k)^{-1}$ is the inverse of the Jacobian matrix

$$\mathbf{J}(\mathbf{x}) \equiv \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

Note the analogy between the scalar $f(x^k)$ in Equation 12 and the vector $\mathbf{f}(\mathbf{x}^k)$ in Equation 13, and the inverse of the derivative $1/f'(x^k)$ in Equation 12 and the inverse of the

matrix of the partial derivatives $J(\mathbf{x}^k)^{-1}$ in Equation 13.

If we replace the step $\mathbf{p}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$ into Equation 13, we obtain

$$\mathbf{p}^{k+1} = -J(\mathbf{x}^k)^{-1} \mathbf{f}(\mathbf{x}^k)$$

or

$$J(\mathbf{x}^k) \mathbf{p}^{k+1} = -\mathbf{f}(\mathbf{x}^k)$$

in which $J(\mathbf{x}^k)$ is a known $(n \times n)$ square matrix, $\mathbf{f}(\mathbf{x}^k)$ is a known n -vector and \mathbf{p}^{k+1} is the vector of n unknowns. In other words, to find the Newton step we have to solve a system of linear equations. Hence, the Newton's algorithm for systems of nonlinear equations is as follows

0. Set $k = 0$; choose tolerance ϵ ; guess \mathbf{x}^0 .
1. Calculate step \mathbf{p}^{k+1} by solving $J(\mathbf{x}^k) \mathbf{p}^{k+1} = -\mathbf{f}(\mathbf{x}^k)$; calculate new point $\mathbf{x}^{k+1} = \mathbf{x}^k + \mathbf{p}^{k+1}$.
2. If $f_i(\mathbf{x}^{k+1}) < \epsilon$ for all i , stop: \mathbf{x}^{k+1} is the solution; otherwise, set $k = k + 1$ and go to 1.

Example 1: System of two equations

We want to solve the following system of two equations

$$\begin{aligned} f_1(x_1, x_2) &= 2x_1^2 + x_2^2 - 5 = 0 \\ f_2(x_1, x_2) &= x_1 + 2x_2 - 3 = 0 \end{aligned} \quad (14)$$

starting at $\mathbf{x}^0 = [1.5 \quad 1.0]^T$ and using $\epsilon = 10^{-4}$.

Solution

At $\mathbf{x}^0 = [1.5 \quad 1.0]^T$, we calculate $\mathbf{f}(\mathbf{x}^0) = [0.5 \quad 0.5]^T$, which means that \mathbf{x}^0 is not a solution. First, we determine the Jacobian

$$J(\mathbf{x}) = \begin{bmatrix} 4x_1 & 2x_2 \\ 1 & 2 \end{bmatrix}$$

Iteration $k = 0$.

Step 1. At \mathbf{x}^0 we calculate $J(\mathbf{x}^0) = \begin{bmatrix} 6 & 2 \\ 1 & 2 \end{bmatrix}$ and solving $\begin{bmatrix} 6 & 2 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} p_1^1 \\ p_2^1 \end{bmatrix} = -\begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$, we determine the first step $\mathbf{p}^1 = [0 \quad -0.25]^T$ and the next point $\mathbf{x}^1 = [1.5 \quad 0.75]^T$.

Step 2. At $\mathbf{x}^1 = [1.5 \quad 0.75]^T$, we calculate $\mathbf{f}(\mathbf{x}^1) = [0.0625 \quad 0]^T$, i.e. \mathbf{x}^1 is not a solution.

Iteration k	x_1^k	x_2^k	$f_1(\mathbf{x}^k)$	$f_2(\mathbf{x}^k)$	p_1^{k+1}	p_2^{k+1}
0	1.5000	1.0000	0.5000	0.5000	0.0000	0.2500
1	1.5000	0.7500	0.0625	0.0000	-0.0119	0.0595
2	1.4881	0.7559	3.2×10^{-4}	0.0000	-6.1×10^{-4}	3.1×10^{-5}
3	1.4889	0.7560	6.7×10^{-6}	0.0000	-0.1×10^{-6}	0.0000

Table 2: Iterations of Newton's method.

Iteration $k = 1$.

Step 1. At \mathbf{x}^1 we calculate $\mathbf{J}(\mathbf{x}^1) = \begin{bmatrix} 6 & 1.5 \\ 1 & 2 \end{bmatrix}$, and solving the corresponding system of linear equations, we get $\mathbf{p}^2 = -\begin{bmatrix} 0.11905 & 0.00595 \end{bmatrix}^T$ and $\mathbf{x}^2 = \begin{bmatrix} 1.4881 & 0.75595 \end{bmatrix}^T$.

Step 2. We calculate $\mathbf{f}(\mathbf{x}^2) = \begin{bmatrix} 0.00032 & 0 \end{bmatrix}^T \neq \begin{bmatrix} 0 & 0 \end{bmatrix}^T$. So we have to continue.

The solution of this problem is $\mathbf{x}^* = \begin{bmatrix} 1.4889 & 0.7560 \end{bmatrix}^T$, and is found after four iterations if the tolerance is $\epsilon = 10^{-4}$ (see Table 2). \square

5 Process Design Example

Equipped with Newton's method, we can now try to find the flows in the process in Figure 1. We are given the following data

1. The molecular weights of the three compounds are: $M_A = 78$, $M_B = 70$, and $M_C = 148$. The common density can be assumed to be $\rho = 1000 \text{ kg/m}^3$.
2. The equilibrium constant K_{eq} at the specified temperature and pressure is equal to $4.45 \text{ (m}^3/\text{kmol)}$.
3. The separation in the flash tank is sharp: product C is fully recovered in the liquid stream (i.e. $\phi_C = 0.0$), and raw materials are fully recovered in the vapor stream (i.e. $\phi_A = 1.0$ and $\phi_B = 1.0$).

As you will see later, the process in Figure 1 corresponds to many different process designs. Here we study a special case, where we are given the following inputs and specifications:

1. There is no C in stream S_1 . The flows of raw materials A and B are 10 and 12 kmol/hr, respectively.
2. We are also told that we should find a design that produces 9.5 kmol/hr of C.

Before using the computer to solve the flowsheet, it is helpful to first enumerate the unknowns and equations to decide if the problem is well posed.

Unknowns. We have the molar flows $N_j^{S_k}$ for $j = \{A, B, C\}$, $k = 1, \dots, 7$ giving 21 unknown molar flows. In expressing the unit balances we introduced two new unknowns, the reaction extent ξ and recycle ratio, R , giving a total of 23 unknowns.

Equations. The mixer balance gives 3 equations, the reactor gives 4, the flash tank gives 6, and the splitter gives 6 for a total of 19 equations. The problem statement also defines the feed flows ($N_j^{S_1}$, $j \in \{A, B, C\}$) for 3 more equations and the production rate of C ($N_C^{S_5}$) for one more equation giving 23 equations.¹ The problem should be well posed and ready to be solved.

6 Exercises

Exercise 1: Code your own Newton method

Write your own MATLAB code to find the root of Equation 10, $f_1(x) = x^3 - 2x^2 + 3x - 6 = 0$ using Newton's method. Try different initial points. Do you find the same root? Plot $f_1(x)$ for $x \in [-2, 3]$.

Exercise 2: $f_2(x) = x^3 - 3x - 2 = 0$

Modify your code for Exercise 1 to solve $f_2(x) = x^3 - 3x - 2 = 0$. Try different initial points again. Do you now find different roots? How many?

Exercise 3: $f_3(x) = x^3 - 2x^2 - x + 2 = 0$

Repeat Exercise 2 for solving $f_3(x) = x^3 - 2x^2 - x + 2 = 0$. Try different starting points. How many roots do you find? What is going on? Plot functions $f_2(x)$ and $f_3(x)$ for $x \in [-2, 3]$.

Exercise 4: MATLAB's `fsolve` function

Use MATLAB's `fsolve` to solve the system in Equation 14. Try different initial points.

Exercise 5: Solve the flowsheet

Develop a model in MATLAB for the process in Figure 1. Solve it using `fsolve`.

Exercise 6: Production rate versus recycle ratio and best economic operation

Consider the flowsheet of Figure 1.

- (a) Vary the recycle ratio, R , and plot the production rate of C and Q^{S_3} versus R for $0 \leq R < 1$. What production rate is achieved without recycle? What is the largest production rate that can be achieved with this process?

¹We could also choose to include Q^{S_3} as an unknown and count Equation 5 as an equation to obtain 24 unknowns and 24 equations. This choice would not change the tentative conclusion that the problem is well posed and ready to be solved.

- (b) Examine the Q^{S_3} versus R plot. Discuss the competing factors in selecting R for the best economics of this process. What R do you expect to be near the economic optimum for this process?

Exercise 7: Process flowsheet with nonsharp separation

- (a) Repeat Exercise 6 with the separation factors changed to

$$\phi_A = 0.8 \quad \phi_B = 0.9 \quad \phi_C = 0.2$$

Assume the production rate of C is the molar flow in S_5 only and you cannot recover the C in S_6 . Does production rate go up or down compared to the sharp separation case considered in Exercise 6? How much C is lost in S_6 ?

- (b) How has the economic situation changed with respect to choosing the recycle ratio for this case compared to the sharp separation case considered in Exercise 6? What value of R do you expect to be near the economic optimum for this process?

Exercise 8: Flowsheet example with ideal mixture equation of state and nonconstant mass density

Let's consider the case in which the mixture density varies with composition. The simplest equation of state to use in modeling this dependence comes from treating the mixture as a so-called ideal mixture.² In an ideal mixture, the volume of a mixture of components is the sum of the volumes occupied by the pure components comprising the mixture; for the (A,B,C) mixture we have

$$n_A V_A^0 + n_B V_B^0 + n_C V_C^0 = V \quad \text{ideal mixture, volumes of components add}$$

in which V_j^0 is the specific volume (vol/mol) of pure component j , which can also be expressed in terms of the mass density and molecular weight

$$V_j^0 = \frac{M_j}{\rho_j^0}$$

Dividing the ideal mixture equation by V and using the mass density in place of specific volume gives

$$\sum_j c_j \frac{M_j}{\rho_j^0} = 1$$

We can multiply this equation by the volumetric flowrate to obtain a relation between volumetric flowrate and molar flows for all streams in the process

$$Q^{S_k} = \sum_j N_j^{S_k} \frac{M_j}{\rho_j^0} \quad \text{ideal mixture} \quad (15)$$

²You will learn more general equations of state in the CBE 311 course.

Notice if the pure component densities are all equal ($\rho_j^0 = \rho^0$), then we can factor that term out of the sum and we have the relation that we used previously to calculate the volumetric flowrate out of the reactor

$$Q^{S_k} = \frac{\sum_j N_j^{S_k} M_j}{\rho^0} \quad \text{constant density assumption} \quad (16)$$

If we want to know the mass density of each stream, we can calculate it from the molar concentration and molecular weights by $\rho^{S_k} = \sum_j c_j^{S_k} M_j$. If we have found the $N_j^{S_k}$, then we can compute ρ^{S_k} using this equation and the previous equation for Q^{S_k}

$$\rho^{S_k} = \sum_j c_j^{S_k} M_j = \frac{\sum_j N_j^{S_k} M_j}{Q^{S_k}}$$

$$\rho^{S_k} = \frac{\sum_j N_j^{S_k} M_j}{\sum_j N_j^{S_k} \frac{M_j}{\rho_j^0}}$$

- (a) Compute the production rate of C as a function of recycle ratio $0 \leq R < 1$ using the constant density assumption with

$$\rho^0 = 1000 \text{ kg/m}^3$$

and the other parameters given in Exercise 4. Plot production rate of C versus R for this case. Note that this program uses Equation 16 for the reactor volumetric flowrate Q^{S_3} .

- (b) Replace Equation 16 in your program with Equation 15 and resolve the problem using the ideal mixture equation of state with pure component densities given by

$$\left[\rho_A^0 \quad \rho_B^0 \quad \rho_C^0 \right] = \left[800 \quad 900 \quad 1100 \right] \text{ kg/m}^3$$

Plot production rate of C versus R for this case.

- (c) Compute and plot the fractional error in the C production rate versus recycle ratio. Is the constant density assumption a reasonable assumption for this problem?
- (d) For $R = 0.6$, compute Q^{S_k} and ρ^{S_k} for all seven streams $i = 1, \dots, 7$. Print out and clearly label these values. What are their values for the constant density case?

Exercise 9: A second reaction

Consider again the process flow diagram of Module 4 shown in Figure 3, but consider the case of two reactions



in which K_1 and K_2 are the equilibrium constants for the two reactions. Both reactors are assumed to be at equilibrium and you may assume constant density for the mixture. The parameter values are

$$M = [78 \ 70 \ 148 \ 218] \text{ kg/kmol} \quad \phi = [0.8 \ 0.9 \ 0.15 \ 0.1]$$

$$N_f = [10 \ 18 \ 0 \ 0] \text{ kmol/hr} \quad K = [2 \ 0.2] \text{ m}^3/\text{kmol} \quad \rho = 1000 \text{ kg/m}^3$$

We wish to manufacture product C, and reaction 2 is regarded as an unwanted side reaction that converts our desired product into an undesired side product D. Define the conversions of A and B to be

$$x_A = \frac{N_A^{S_1} - (N_A^{S_6} + N_A^{S_5})}{N_A^{S_1}} \quad x_B = \frac{N_B^{S_1} - (N_B^{S_6} + N_B^{S_5})}{N_B^{S_1}}$$

Define the yields of C and D to be

$$y_C = \frac{N_C^{S_5}}{N_C^{S_5} + N_D^{S_5}} \quad y_D = \frac{N_D^{S_5}}{N_C^{S_5} + N_D^{S_5}}$$

- (a) Solve for the steady state as a function of recycle ratio in the range $0 \leq R \leq 1$. Make three plots: $N_C^{S_5}$ and $N_D^{S_5}$ (production rates) versus R ; y_C and y_D versus R ; and x_A and x_B versus R .
- (b) Given your plots, answer the following three questions

1. If you wish to maximize the yield of C, what recycle ratio do you use?
2. If you wish to maximize the conversion of A, what recycle ratio do you use?
3. If you wish to maximize production rate of C, what recycle ratio do you use?

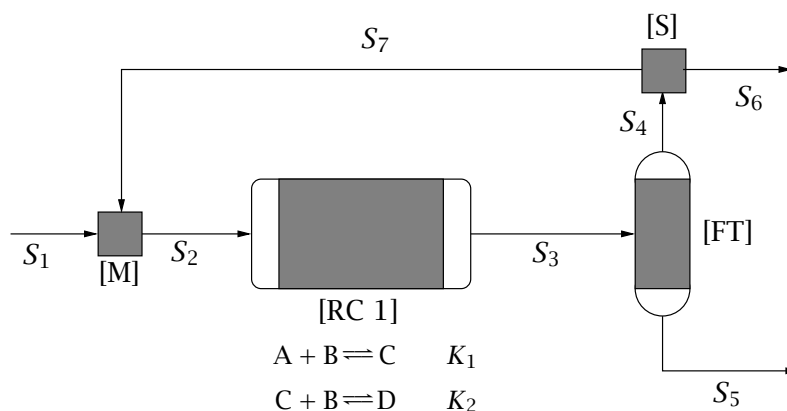


Figure 3: Process flow diagram for the production of C with two reactions.

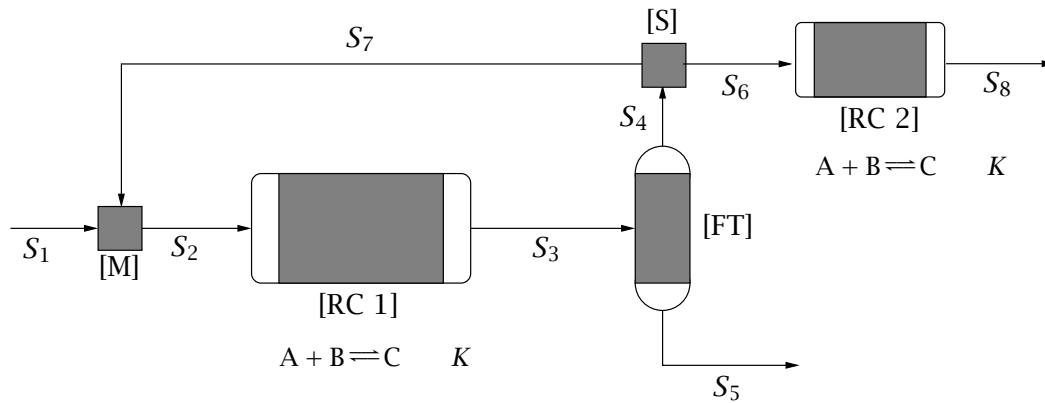


Figure 4: Process flow diagram for the production of C with an additional reactor.

- (c) These three objectives all seem like reasonable plant objectives. Discuss why these objectives lead to different operations. Which operation would you choose? Justify your answer.

Exercise 10: A single reaction but a second reactor

Consider now a single reaction as in Module 4, but a second *reactor* shown in Figure 4. The parameter values are the same as the sharp separation case considered in Module 4

$$M = [78 \quad 70 \quad 148] \text{ kg/kmol} \quad \phi = [1.0 \quad 1.0 \quad 0]$$

$$N_f = [10 \quad 12 \quad 0] \text{ kmol/hr} \quad K = 4.45 \text{ m}^3/\text{kmol} \quad \rho = 1000 \text{ kg/m}^3$$

- (a) Add the second reactor to your flowsheet model and solve for the steady state over the range of recycle ratios $0 \leq R \leq 1$. You should add unknowns: ξ_2 , Q^{S_8} , and $N_{A,B,C}^{S_8}$, and appropriate reactor equations to include the second reactor in the model.

Plot production rate of C, which is now $N_C^{S_5} + N_C^{S_8}$, versus R in one figure. Plot flowrates Q^{S_3} versus $N_C^{S_5}$ (*not* R) in a second figure for this two-reactor case.

- (b) Change your set of equations so that $\xi_2 = 0$ in the second reactor is the solution, and solve the flowsheet again. Since you are not allowing any reaction in the second reactor, N^{S_8} should be equal to N^{S_6} and you should get the same results as in Exercise 6 of Module 4. This is the one-reactor case.

Plot production rate of C, $N_C^{S_5}$, versus R in one figure, and flowrate Q^{S_3} versus $N_C^{S_5}$ (*not* R) in a second figure for this single reactor case.

- (c) Comparing these two cases, if you want to produce C at rate 9.995 kmol/hr, what recycle ratio do you use with a single reactor. What recycle ratio do you use with two reactors. Discuss the advantages and disadvantages of these two different designs.