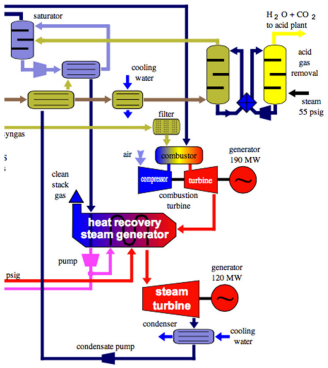
Chapter 3



Introduction to Material Balance & Single Unit Process Material Balance Calculations

Course Learning Outcomes

At the end of this course students will be able to

- define a system and draw the system boundaries for which the material balance is to be made.
- draw and fully label a flowchart
- choose a convenient basis of calculation
- perform the degree of freedom analysis
- write in order the equations used to calculate specific process variables
- perform material balance calculations on a single unit process

Process Classification

- **Classification of processes**
  - **Batch** : feed is charged, products are removed some time later
  - **Continuous** : inputs and outputs flow continuously
  - **Semi batch** process : semi continuous process
- **Condition of processes**
  - **Steady state** : process variables do not change with time
  - **Transient (unsteady) state** : process variables change with time
- **Usage of processes**
  - Batch processing is for relatively small quantity of products
  - Continuous processing is better suited to large production rates.

Material Balance

q_{in}(kg CH_4/h) → **SYSTEM** → q_{out} (kg CH_4/h)

- Suppose methane is a component of both the input and output streams of a continuous process unit but the mass flow rates of methane in both streams are measured and found to be different.
- There are four possible explanations for the observed difference?

General Balance Equation

- **Input - Output + Generation - Consumption = Accumulation**
  - **Input** : Enters through system boundaries
  - **Output** : Leaves through system boundaries
  - **Generation** : Produced within the system
  - **Consumption** : Consumed within system
  - **Accumulation** : Buildup within system

Types of Balances

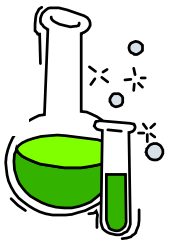
- **Differential Balances**
  - √ Indicate what is happening in the system at an instant of time
  - √ Each term of the balance equation is then a rate (eg: flow rate)
  - √ Unit: balanced quantity unit divided by a time unit (kg SO_2/hr)
- **Integral Balances**
  - √ Describe what happens between two instants of time.
  - √ Each term of the equation is then amount of the balanced quantity
  - √ Unit: amount of quantity (kg SO_2)
  - √ Normally applied to batch process

→ **Steady state balance**
  - √ No accumulation term

Integral Balances on Batch Process

Recall:

$Input_{initial}$ - $Output_{final}$ + Generation – Consumption = Accumulation



Integral Balances on Batch or Semi-batch Processes

- Integral balance on batch processes
  - ✓ Sometimes it can be treated like steady-state processes
- Integral balance on Semi-batch and continuous process
  - ✓ Sometimes it can be easily solved.
  - ✓ Require integration over period of time

- General material balance

  Input - Output + Generation - Consumption = Accumulation

- For steady state, accumulation = 0

$$\text{accumulation} = \frac{dy}{dt} = 0$$

  - Then ; **Input - Output = Generation – Consumption**
  - If **NO** reaction; **Input = Output**

- Objective :

  Given values of input, output → calculate unknown values

- Flow Charts : simple way to visualize process flow

  - ✓ **PFD (Process flow diagram)**
  - ✓ **P&ID (Process and Instrumentation diagram)**

1) Draw a flow chart and specify your boundary. Fill in all given values.
2) Choose as a basis of calculation an amount or flow rate of one of the process streams.
3) Label unknown stream variables on the chart.
4) Do the problem bookkeeping. (# unknowns, # independent equations & degree of freedom analysis)
5) Convert volume flow rates to mass or molar flow rates.
6) Convert mixed mass and molar flow rates to mass or molar flow rates.
7) Translate given information to equations.
8) Write material balance equations.
9) Solve equations.
10) Scale up/down.

Process Description

The catalytic dehydrogenation of propane is carried out in a continuous packed bed reactor. One thousand pounds per hour of pure propane are fed to preheater where they are heated to a temperature of 670°C before they pass into the reactor. The reactor effluent gas, which includes propane, propylene, methane and hydrogen, is cooled from 800°C to 110°C and fed to an absorption tower where the propane and propylene are dissolved in oil. The oil then goes to a stripping tower in which it is heated, releasing the dissolved gases; these gases are recompressed and sent to a high pressure distillation column in which the propane and propylene are separated. The product stream from the distillation column contains 98% propylene, and the recycle stream is 97% propane. The stripped oil is recycled to the absorption tower.

Complex, not easy to understand

Gas containing N_2 and O_2 is combined with propane in a batch combustion chamber in which some (but not all) of the O_2 and C_3H_8 react to form CO_2 and H_2O. and the product is then cooled, condensing water. The flowchart is given below:

Write the values and units of all known stream variables at the locations of the streams on the chart.

Example: A stream containing 21 mol % O_2 and 79 mol % N_2 at 320˚C and 1.4 atm flowing at the rate of 400 mol/h might be labeled :

The information can be given in two ways: as the total amount or flow rate of the stream and the fractions of each component:

1. Amount or Flow rate of each component

2. Flow rate of the stream and the fractions of each components

Assign* algebraic symbols to unknown stream variables** (such as *Q* kg solution/min, *x* kg N_2/kg, *n* kmol C_3H_8, etc.) and ***write these variable names and their associated units on the chart .

Unknown : flow rate
Known: fraction

Unknown : fraction
Known: flow rate

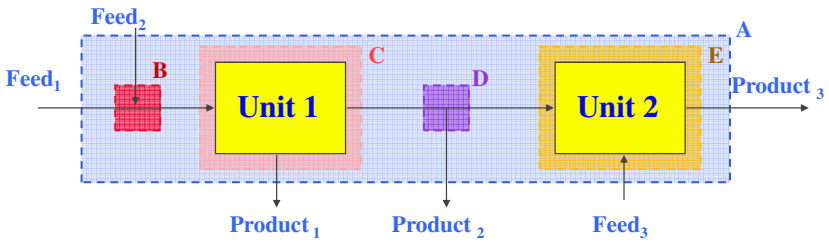
Air Humidification and Oxygenation Process

An experiment on the growth rate of certain organisms requires the establishment of an environment of humid air enriched in oxygen. Three inputs streams are fed into an evaporation chamber to produce an output stream with the desired composition

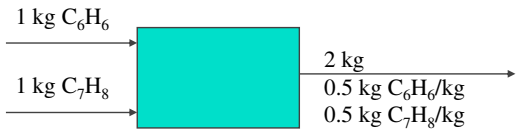
A: Liquid water, fed at a rate of 20.0 cm^3/min.
B: Air (21 mol% O_2, the balance N_2).
C: Pure O_2, with a molar flow rate 1/5 of the molar flow rate of stream B.

The output gas is analyzed and is found to contain 1.5 mole% water. Draw and label flowchart of the process, and calculate all unknown stream variables.

Please work on 'TEST YOURSELF' questions in page 93)

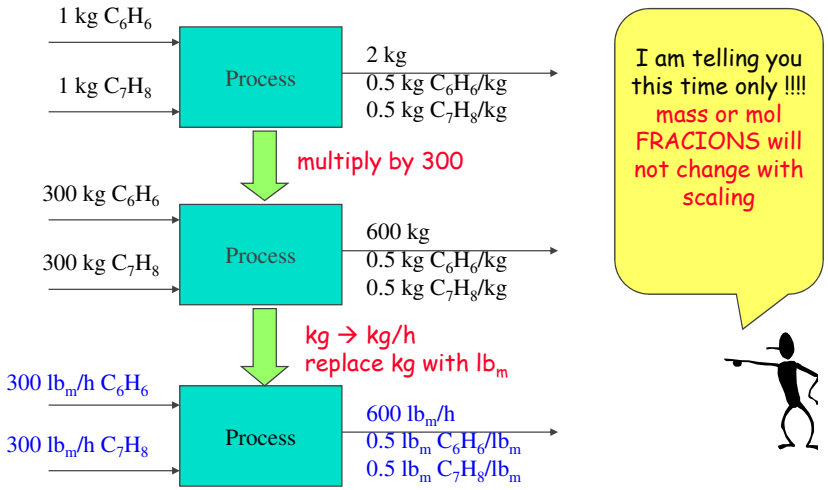


- Boundary system
  - ✓ System (overall balance) ……. Boundary A (3 inputs, 3 outputs)
  - ✓ Sub-system (balance on each process unit)
    - – Stream mixer …… Boundary B (2 inputs, 1 output)
    - – Unit 1 (e.g. reactor) ……Boundary C (1 input, 2 outputs)
    - – Splitter …… Boundary D (1 input, 2 outputs)
    - – Unit 2 (e.g. mixer) …… Boundary E (2 inputs = 1 output)



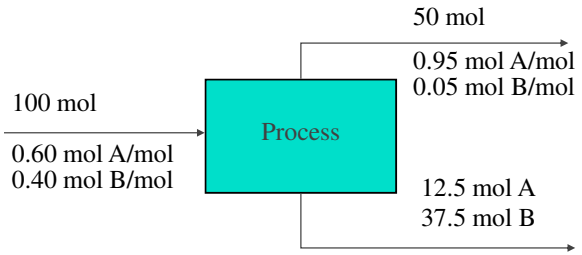
- The process is **balanced**, since material balances on both system components C_6H_6 and C_7H_8 are satisfied [1 kg in = (2 x 0.5) kg out in both cases]
- Masses (but not the mass fractions) of all streams could be multiplied by a common factor and the process remain balanced
- This procedure of multiplication is referred as scaling the flowchart
  - ✓ **scaling up** – final stream quantities are larger than original quantities
  - ✓ **scaling down** - if they are smaller

Flowchart Scaling and Basis of Calculation



Scale-up of a Separation Process Flowchart

A 60-40 mixture (by moles) of A and B is separated into two fractions. A flowchart of the process is shown. It is desired to achieve the same separation with a continuous feed of 1250 lb-moles/h. Scale the flowchart accordingly.



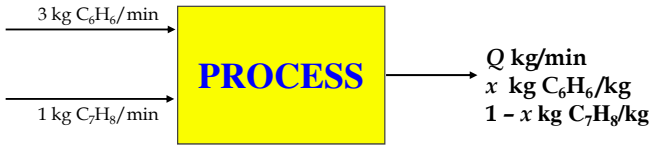
Scale-up of a Separation Process Flowchart

Basis of Calculation

- The first step is to choose an amount (mass or moles) or a mass or molar flowrate of a stream as a basis of calculations
  - ✓ The input flowrate: 100 mol/h CO_2
  - ✓ The production of 5 kg/h of product.
- If a stream amount or flow is given in a problem statement, it is usually most convenient to use this quantity as a **basis of calculations**
  - ✓ all unknown variables are then determined to be consistent with this basis
  - ✓ For rule of thumbs for process with no reaction :
    - mass is normally use with liquid
    - number of mol is use for gas
- If no stream amounts or flow rates are known, assume one preferably with that of a stream with a known composition

Problem

Suppose that 3 kg/min of Benzene and 1 kg/min of Toluene are mixed. Assuming the process is at steady state the process flowchart might be drawn and labeled as shown:



and for steady state process with no reaction, the general material balance equation becomes

Input = Output

There are two unknown quantities, Q and x, associated with the process.

"The maximum number of independent equations that can be derived by writing balances on a non-reactive system equals the number of chemical species in the input and output streams" ***… pg 96 (text book)***

So three possible balances can be written, i.e. total, benzene and toluene. Any two of which can be used to determine Q and x, for example ;

Problem

Two methanol-water mixtures contained in separate flasks. The first mixture contains 40 wt% methanol, and the second contains 70 wt% methanol. If 200 g of the mixture are combined with 150 g of the second, what are the mass and composition of the product?

100.0 kg/hr of a liquid mixture of benzene (B) and toluene (T) that contains 55% benzene by mass is partially evaporated to yield m_v (kg/h) of a vapor containing 85.0% benzene and m_l (kg/h) of a residual liquid containing 89.4% toluene by mass. The operation is continuous and at steady state.

1. Draw a process flowchart
2. Write balances on total mass and on benzene
3. Determine the expected values of m_v and m_l.

#df = (number of species) - (number of independent equations)

Case 1 (exactly determined – exactly specified)
- If *#df* = 0, Solution is unique
- Process is exactly specified

$$x + y = 3$$
$$2x + y = 4$$
#df = 0

Case 2 (underdetermined – underspecified)
- If *#df* > 0, There are a lot of solutions.
- Process is underspecified by *#df* equation

$$x + y + z = 3$$
$$2x + y = 4$$
#df = 1

Case 3 (over determined – over specified)
- If *#df* < 0, No solution for this system.
- Process is over specified by *#df* equation

$$x + y = 3$$
$$2x + y = 4$$
$$x + 2y = 3$$
#df = -1

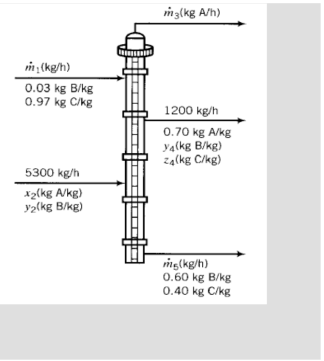
- Material balances
  - ✓ No. of species (*N*) = No. of independent equations for nonreactive process
- An energy balance
  - ✓ One unknown (T, Q, or m)
- Process specification
  - ✓ Requirement (based on economics,…)
- Physical properties and laws
  - ✓ Thermodynamic relations and physical properties data e.g.. $PV = nRT$
- Physical constraints
  - ✓ $x_1 = 1$ then $x_2 = 1 - x_1$, …

The following flowchart shows a distillation column with two feed streams and three product streams

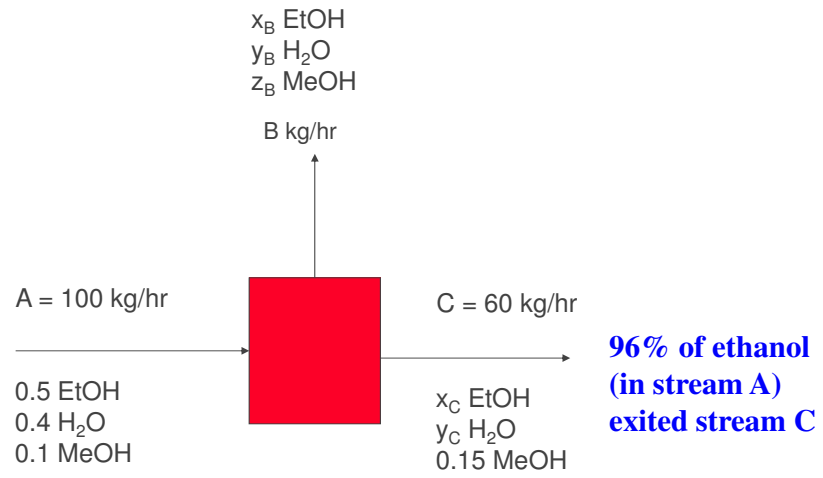
a) How many independent material balances may be written for this system?

b) How many unknowns may be written for this system?

c) How many of the unknown flow rates and/or mole fractions must be specified before the others may be calculated? *(Remember what you know about the component mole fractions of a mixture—for example, the relationship between x_2 and y_2)*



Degrees of Freedom



96% of ethanol (in stream A) exited stream C

Outline of a Procedure for Material Balance Calculations

1) Draw a flow chart and specify your boundary. Fill in all given values.
2) Choose as a basis of calculation an amount or flow rate of one of the process streams.
3) Label unknown stream variables on the chart.
4) Do the problem bookkeeping. (# unknowns, # independent equations & degree of freedom analysis)
5) Convert volume flow rates to mass or molar flow rates.
6) Convert mixed mass and molar flow rates to mass or molar flow rates.
7) Translate given information to equations.
8) Write material balance equations.
9) Solve equations.
10) Scale up/down.

Material Balances on a Distillation Column

A mixture containing 45% benzene (B) and (55%) toluene (T) by mass is fed to a distillation column. An overhead stream 95 wt% B is produced, and 8% of the benzene fed to the column leaves in the bottom stream. The feed rate is 2000 kg/h. Determine the overhead flow rate and the mass flow rates of benzene and toluene in the bottom stream.

Solution

1. Basis: Given Feed rate
2. Draw flowchart and label it
3. Label unknown stream variables on the chart. Write the relationship between known and unknown variable (e.g. Contains "8 % of the B in the feed").

Balances on a Distillation Column Example 4.3-5 in textbook (pg. 102)

(4) Do the problem book keeping.
- How many unknowns?
- How many independent equations?
- If the numbers are equal, the problem can in principal be solved