Fondamenti dell’ingegneria di processo

anno accademico 2021-2022

Fundamentals of material balances

Certain restrictions imposed by nature must be taken into account when designing a new process or analyzing an existing one.
You cannot, for example, specify an input to a reactor of 1000 g of lead and an output of 2000 g of lead.

The basis for this observation is the
law of conservation of mass,
which states that mass can neither be created nor destroyed

Statements based on the law of conservation of mass such as
"total mass of input = total mass of output"
or
"(g sulfur/day)in = (g sulfur/day)out"
are examples of **mass balances** or **material balances**.

The design of a new process or analysis of an existing one is not complete until it is established that the inputs and outputs of the entire process and of each individual unit satisfy balance equations.

Fundamentals of material balances

Given a process description, you should be able to do the following:

a) draw and fully **label** a flowchart;

b) for a multiple-unit process, identify the subsystems for which balances might be written;

c) perform the **degree-of-freedom analysis**

d) choose a convenient **basis of calculation**;

e) write in order the **equations** you would use to calculate specified process variables;

f) perform the calculations.

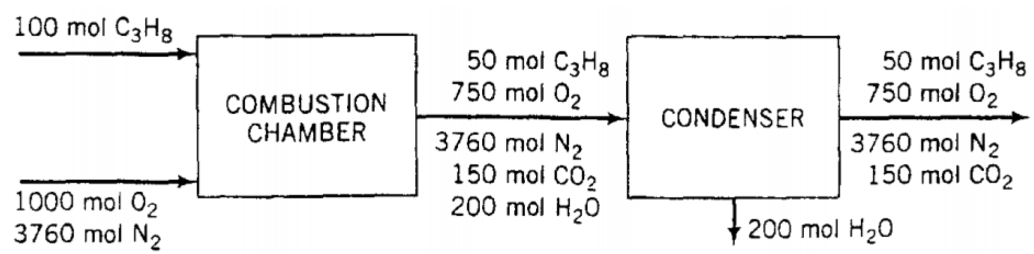
You should be able to do these computations for single-unit and multiple-unit processes.

Fundamentals of material balances

Labelling a flowchart

When you are given process information and asked to determine something about the process, it is essential to organize the information in a way that is convenient for subsequent calculations.
The best way to do this is to draw a **flowchart** of the process, using boxes or other symbols to represent process units (reactors, mixers, separation units, etc.) and lines with arrows to represent inputs and outputs.

Used properly, the flowchart of a process can help get material balance calculations started and keep them moving. To do so, the chart must be fully **labeled** when it is first drawn, with *values of known process variables* and *symbols for unknown variables being written for each input and output stream*.
Thereafter, the chart functions as a scoreboard for the problem solution: as each unknown variable is determined its value is filled in, so that the chart provides a continuous record of where the solution stands and what must still be done.



Labeled flowchart of a combustion-condensation process

Fundamentals of material balances

Labelling a flowchart

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

For example, a stream containing 21 mole% O2 and 79% N2 at 320°C and 1.4 atm flowing at a rate of 400 mol/h might be labeled

$$\xrightarrow{\text{400 mol/h}}$$

0.21 mol O_2/mol
0.79 mol N_2/mol
T = 320°C, P = 1.4 atm

The stream variables of primary interest in material balance problems are those that indicate how much of each component is present in the stream (for a batch process) or the flow rate of each component (for a continuous process).

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

$\longrightarrow$	$\Longleftrightarrow$	$\xrightarrow{\text{100 kmol/min}}$
60 kmol N_2/min		0.6 kmol N_2/kmol
40 kmol O_2/min		0.4 kmol O_2/kmol

Fundamentals of material balances

Labelling a flowchart

2. ***Assign algebraic symbols to unknown stream variables [such as m (kg solution/min), x (g N2/g), and n (kmol C3H8/h] and write these variable names and their associated units on the chart.***

For example, if you did not know the flow rate of the stream described in the first illustration of step 1, you might label the stream

$\dot{n}$(mol/h)

$\longrightarrow$

0.21 mol O_2/mol
0.79 mol N_2/mol
$T = 320°C$, $P = 1.4$ atm

while if the flow rate were known and the mole fractions were not, the stream might be labeled

400 mol/h

$\longrightarrow$

y(mol O_2/mol)
$(1 - y)$(mol N_2/mol)
$T = 320°C$, $P = 1.4$ atm

Fundamentals of material balances

Labelling a flowchart

An extraction-distillation process

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams one enriched in acetone, the other in water. The separation process consists of extraction of the acetone from the water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water.

The description that follows introduces some of the terms commonly used in reference to liquid extraction processes.

The acetone (solute)-water (diluent) mixture is first contacted with the MIBK (solvent) in a mixer that provides good contact between the two liquid phases. A portion of the acetone in the feed transfers from the aqueous (water) phase to the organic (MIBK) phase in this step. The phase rich in the diluent (water, in this process) is referred to as the raffinate, and the phase rich in the solvent (MIBK) is the extract. The mixer-settler combination is the first stage of this separation process.

The raffinate passes to a second extraction stage where it is contacted with a second stream of pure MIBK, leading to the transfer of more acetone. The two phases are allowed to separate in a second settler, and the raffinate from this stage is discarded. The extracts from the two mixer-settler stages are combined and fed to a distillation column.

The overhead effluent is rich in acetone and is the process product. The bottom effluent is rich in MIBK and in a real process would be treated further and recycled back to the first extraction stage, but we will not consider recycle in this example.

In a pilot-plant study, for every 100 kg/h of acetone-water fed to the first extraction stage, 100 kg/h of MIBK is fed to the first stage and 75 kg/h is fed to the second stage. The extract from the first stage is found to contain 27.5 wt% acetone. The second-stage raffinate has a flowrate of 43.1 kg/h and contains 5.3 wt% acetone, 1.6 wt% MIBK, and 93.1 wt% water, and the second-stage extract contains 9.0% acetone, 88.0 wt% MIBK, and 3.0 wt% water. The overhead product from the distillation column contains 2.0 wt% MIBK, 1.0% water, and the balance acetone.

Fundamentals of material balances

Labelling a flowchart

Propylene production by dehydrogenation of propane

The catalytic dehydrogenation of propane is carried out in a continuous packed bed reactor. One thousand kilograms per hour of propane is preheated to a temperature of 670 °C before it passes 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 sent to a distillation column in which the propane and propylene are separated.

The propane stream is recycled back to join the feed to the reactor preheater. The top product stream from the distillation column contains 98 wt% propylene, and the recycle stream is 97 wt% propane.

The stripped oil is recycled to the absorption tower.

Fundamentals of material balances

Degree-of-Freedom Analysis

Single-unit processes

To perform a degree-of-freedom analysis, draw and completely label a flowchart, count the unknown variables on the chart, then count the independent equations relating them, and subtract the second number from the first.
There are three possibilities:

1. If $\mathbf{n_{Dof} = 0}$, there are n independent equations in n unknowns and the problem can in principle be solved.
2. If $\mathbf{n_{Dof} > 0}$, there are more unknowns than independent equations relating them, and at least dof additional variable values must be specified before the remaining variable values can be determined. Either relations have been overlooked or the **problem** is **underspecified** and has infinitely many solutions; in either case, plunging into calculations is likely to be a waste of time.
3. If $\mathbf{n_{Dof} < 0}$, there are more independent equations than unknowns. Either the flowchart is incompletely labeled or the problem is **overspecified** with redundant and possibly inconsistent relations. Again there is little point wasting time trying to solve it until the equations and unknowns are brought into balance.

Fundamentals of material balances

Single-unit processes

nonreactive processes

Degree-of-Freedom Analysis

Sources of equations relating unknown process stream variables include the following:

Material balances. For a **nonreactive process**, no more than *n* independent material balances may be written, where n is the number of molecular species involved in the process.
For example, if benzene and toluene are the species in the streams entering and leaving a distillation column, you could write balances on benzene, toluene, total mass, atomic carbon, atomic hydrogen, and so on, but at most two of those balances would be independent. If additional balances are written, they will not be independent of the first ones and so will provide no new information. For a reactive process, the procedure becomes more complicated.
An energy balance. If the amount of energy exchanged between the system and its surroundings is specified or if it is one of the unknown process variables, an energy balance provides a relationship between inlet and outlet material flows and temperatures.
Process specifications. The problem statement may specify how several process variables are related. For example, you may be told that of the acetone fed to a condenser [flow rate = m1 (kg acetone/s)], 40% appears in a condensate stream [flow rate = m2 (kg acetone/s)]. A system equation would then be m2 = 0.40 m1. 4.
Physical properties and laws. Two of the unknown variables may be the mass and volume of a stream material, in which case a tabulated specific gravity for liquids and solids or an equation of state for gases would provide an equation relating the variables. In other instances, saturation or equilibrium conditions for one or more of the process streams may provide needed relations.
Physical constraints. For example, if the mole fractions of the three components of a stream are labeled XA, XB, and xc, then a relation among these variables is XA + XB +xc = 1. (If instead of Xc you label the last fraction 1 - x A - XB, then you will have one less variable and one less equation to worry about.)

Fundamentals of material balances

Basis of calculation

Since a balanced process can always be scaled, material balance calculations can be performed on the basis of any convenient set of stream amounts or flow rates and the results can afterward be scaled to any desired extent.

A **basis of calculation** is an amount (mass or moles) or flow rate (mass or molar) of one stream or stream component in a process. The first step in balancing a process is to choose a basis of calculation; all unknown variables are then determined to be consistent with this basis.

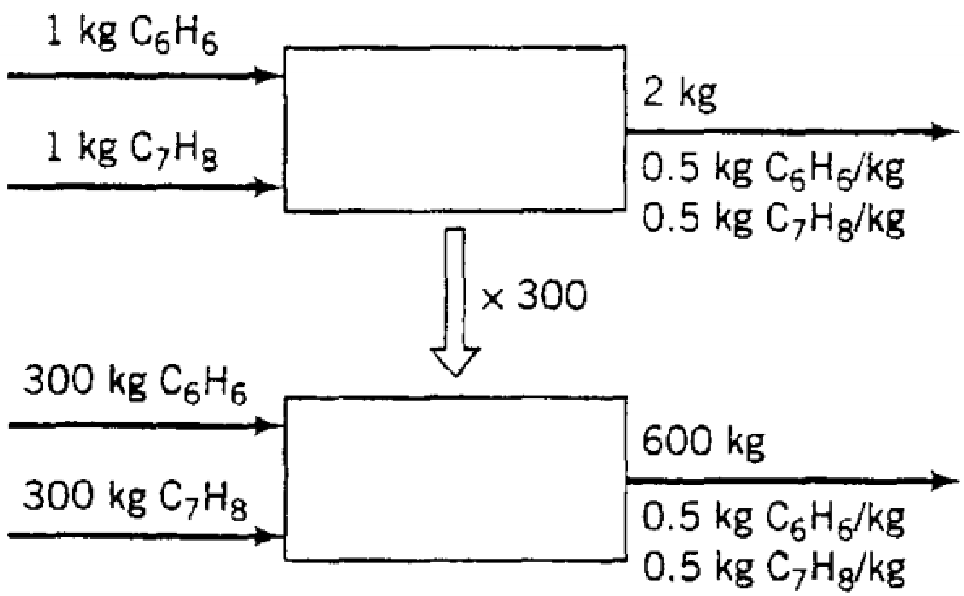
If a flow rate is given in a problem statement, it is usually most convenient to use this quantity as a basis of calculation. If no stream amounts or flow rates are known assume one, preferably that of a stream with a known composition.

The procedure of changing the values of all stream amounts or flow rates by a proportional amount while leaving the stream compositions unchanged is referred to as **scaling** the flowchart - **scaling up** if the final stream quantities are larger than the original quantities, **scaling down** if they are smaller.

Fundamentals of material balances

Scaling

The procedure of changing the values of all stream amounts or flow rates by a proportional amount while leaving the stream compositions unchanged is referred to as **scaling** the flowchart - **scaling up** if the final stream quantities are larger than the original quantities, **scaling down** if they are smaller.



Fundamentals of material balances

Material balance calculations

Example. An experiment on the growth rate of certain organisms requires an environment of humid air enriched in oxygen.

Three input 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 oxygen, with a molar flow rate one-fifth of the molar flow rate of stream B

The output gas is analyzed and is found to contain 1.5 mol% water.

Draw and label a flowchart of the process and calculate all unknown stream variables.

Fundamentals of material balances

Material balance calculations

Example. A feed flowing containing 20 mol% propane (C_3), 30 mol%, isobutane ($i\text{-}C_4$), 20 mol% isopentane ($i\text{-}C_5$) and 30 mol% normal pentane ($n\text{-}C_5$) is separated into two fractions by a distillation column.

The distillate (overhead) contains all of the propane fed to the column, 80% of the isopentane fed, and has a composition that is 40 mol% isobutane.

The bottoms stream contains all of the normal pentane fed to the column.

Draw and label a flowchart, calculate the distillate and bottom flowrates (mol/h), and their compositions (mole fractions).