**KWAME NKRUMAH UNIVERSITY OF SCIENCE AND TECHNOLOGY**

**CHEMICAL ENGINEERING DEPARTMENT**

**CHE 251: CHEMICAL PROCESS CALCULATIONS**

**INSTRUCTOR:** Dr. (Mrs.) Mizpah A. D. Rockson

**LECTURE 7:** Material Balance Calculations

**Learning Objectives**

At the end of the lecture the student is expected to able to understand or do the following:

1. Organize process information into a flowchart
2. Scaling of flowchart
3. Selection of a basis for calculations
4. Balancing non-reactive processes

All material balance problems are variations on a single theme: given values of some input and output stream variables, derive and solve equations for others. Solving the equations is usually a matter of simple algebra, but deriving them from a description of a process and a collection of process data may present considerable difficulties. In this lecture we will outline a procedure for reducing a description of a process to a set of equations that can be solved for unknown process variables.

**7.1 Flowcharts**

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.

For example, suppose a gas containing N2and O2 is combined with propane in a batch combustion chamber in which some (but not all) of the O2 and C3H8 react to form CO2 and H2O, and the product is then cooled, condensing the water. The flowchart of this two-unit process might appear as shown in Figure 7.1



Figure 7.1 Flowchart of a combustion-condensation process.

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.

Several suggestions follow for labeling a flowchart to get the greatest possible benefit from it in material balance calculations.

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 and1.4 atm flowing at a rate of 400 mol/h might be labeled



When you have done this for every stream on the chart, you have a summary of the known information about the process, each item being conveniently associated with the part of the process to which it relates.

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.



1. ***Assign algebraic symbols to unknown stream variables*** [such as (kg solution/min), *x* (Ibm N2/lbm), and *n* (kmol C3H8)] ***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 describedin the first illustration of step 1, you might label the stream,



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



You may ultimately have to derive and solve an equation for each unknown that appears on the chart, and it is therefore to your advantage to keep the number of labeled unknowns to a minimum. When labeling component mass or mole fractions of a stream, for example, variable names need only be assigned to all but one fraction, since the last one must be 1 minus the sum of the others. If you are given that the mass of stream 1 is half that of stream 2, label the masses of these streams *m* and *2m* rather than *ml* and *m2;* if you know that there is three times as much nitrogen (by mass) in a stream as oxygen, label the mass fractions of O2 and N2 *y(g* O2/g) and *3y(g* N2/g) rather than *yl* and *y2.*

If a volumetric flow rate of a stream is given, it is generally useful to label the mass or molar flow rate of this stream or to calculate it directly, since balances are not normally written on volumetric qualities.

***Note on Notation:***Although any symbol may be used to represent any variable, having a consistent notation can aid understanding. In this course, we will generally use *m* for mass, for mass flow rate, *n* for moles, for molar flow rate, *V* for volume, and for volumetric flow rate. Also, we will use *x* for component fractions (mass or mole) in liquid streams and *y* for fractions in gas streams.

***Example 7.1 Flowchart of an Air Humidification and Oxygenation Process***

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 cm3/min

B: Air (21 mole% O2, the balance N2)

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 mole % water. Draw and label a flowchart of the process, and calculate all unknown stream variables.

***Solution***



*Notes on the Labeling:*

1. Since the one known flow rate (20 cm3 H2O/min) is given on a per minute basis, it is most convenient to label all stream flow rates on this basis.

2. Once the variable name is chosen for the air flow rate, the given information about the ratio of the air and O2 flow rates may be used to label the O2 flow rate 0.200 .

3. The mole fractions of the components of any stream must add up to 1. Since the mole fraction of H2O in the outlet stream is known to be 0.015, once the mole fraction of O2 is labeled *y,* that of N2 must be 1 - *(y* + 0.015) = (0.985 - *y)* (mol N2/mol).

The quantity may be calculated from the given volumetric flow rate and the density of liquid water:



The three remaining unknowns ( and *y)* may be determined from balances, all of which have the simple form *input* = *output* for this nonreactive steady-state process. The balances are easily written by referring to the flowchart.





**7.1 Flowchart Scaling and Basis of Calculation**

Suppose a kilogram of benzene is mixed with a kilogram of toluene. The output from this simple process is obviously 2 kg of a mixture that is 50% benzene by mass.



The process depicted by this flowchart is said to be balanced, since material balances on both system components-C6H6 and C7H8-are satisfied. [1 kg in = (2 x 0.5) kg out in both cases.]

Observe now that the masses *(but not the mass fractions)* of all streams could be multiplied by a common factor and the process would remain balanced; moreover, the stream masses could be changed to mass flow rates, and the mass units of all stream variables (including the mass fractions) could be changed from kg to g or Ibm or any other mass unit, and the process would still be balanced.

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.



Suppose you have balanced a process and the amount or flow rate of one of the process streams is *n1.* You can scale the flowchart to make the amount or flow rate of this stream *n2*by multiplying all stream amounts or flow rates by the ratio *n2/n1*.

***Example 7.2 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 here.

It is desired to achieve the same separation with a continuous feed of 1250 lb-moles/h. Scale the flowchart accordingly.



***Solution***

The scale factor is



The masses of all streams in the batch process are converted to flow rates as follows:



The units of the mole fractions in the top product stream may be changed from mol/mol to lb-mole/lb-mole, but their values remain the same. The flowchart for the scaled-up process follows.



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 stream amount or 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. If mass fractions are known, choosea total mass or mass flow rate of that stream (e.g. 100 kg or 100 kg/h) as a basis: if mole fractionsare known, choose a total number of moles or molar flow rate.

**7.3 Balancing a Process**

Suppose 3.0 kg/min of benzene and 1.0 kg/min of toluene are mixed. The process flowchart might be drawn and labeled as follows:



There are two unknown quantities- and *x-*associated with the process, so two equations are needed to calculate them.

Material balance equations for this nonreactive process all have the simple form input = output. Three possible balances can be written-on total mass, benzene, and toluene-any two of which provide the equations needed to determine and *x.*

For example,



The following rules apply to for writing balances for nonreactive processes:

1. *The maximum number of independent equations that can be derived by writing balances on a nonreactive system equals the number of chemical species in the input and output streams.*

In the given example, two substances-benzene and toluene-make up the input and output streams of the process; you can write mass or mole balances on benzene and toluene and a total mass or mole balance, but only two of these three equations are independent-writing the third accomplishes nothing.

1. *Write balances first that involve the fewest unknown variables.*

In the example, a total mass balance involves only one unknown, *,* while benzene and toluene balances each involve both and *x* . By writing first a total balance and then a benzene balance, we were able to solve first one equation in one unknown, then a second equation, also in one unknown. If we had instead written benzene and toluene balances, we would have had to solve two simultaneous equations in two unknowns; the same answers would have been obtained, but with greater effort.

***Example 7.3 Balances on a Mixing Unit***

An aqueous solution of sodium hydroxide contains 20.0% NaOH by mass. It is desired to produce an 8.0% NaOH solution by diluting a stream of the 20% solution with a stream of pure water. Calculate the ratios (liters H2O/kg feed solution) and (kg product solution/kg feed solution).

***Solution***

* Choose a basis of calculation-an amount or flow rate of one of the feed or product streams-and then draw and label the flowchart. We will arbitrarily choose a basis of 100 kg of the 20% feed solution.



* Express what the problem asks you to determine in terms of the labeled variables on the flowchart. The desired quantities are *V1/100* (liters H2O/kg feed solution) and *m2/l00* (kg product solution/ kg feed solution). Our task is therefore to calculate the variables *V1* and *m2.*
* Count unknown variables and equations relating them. If the number of unknowns equals the number of independent equations relating them, you will be able to solve the problem; otherwise, either you have forgotten some relations or the problem is not well defined.

(a) Unknowns. Examining the flowchart, we see three unknown variables- ml, *m2,* and *V1*

(b) Equations. *For a nonreactive process that involves N species, up to N independent material balance equations may be written.* Since there are two species in our process (sodium hydroxideand water), we can write two balances. We could write them on sodium hydroxide, water,total mass, atomic sodium, atomic hydrogen, and so on; the point is that once we have writtenany two, we can obtain no new information by writing a third one.Since we may only write two material balances, we will need a third equation to solve forour three unknowns (m1, *m2,* and *V).* Fortunately, we have one: the mass and volume of thediluent water, ml and *V1*, are related by the density of liquid water, which we know. We thushave three equations in three unknowns and therefore a solvable problem.

* Outline the solution procedure.

All balances for this system have the form *input* = *output.* For example, a total mass balance is 100 kg + *ml* = *m2.* Looking at the flowchart, we can see that balances on total mass and water each involve two unknowns (ml and *m2),* a sodium hydroxide balance only involves one unknown *(m2)* and the water density relationship involves two unknowns (ml and *V1).* We would therefore begin the solution by writing and solving the NaOH balance for *m2,* then writing and solving a total mass or water balance for *m1*, and finally determining *V1* from *m1* and the density.

* NaOH balance (input = output).



* Total mass balance (input = output).



* Diluent water volume. Although we are not given the temperature or pressure at which the mixing is done, the density of liquid water is approximately constant at 1.00 kg/liter. We may therefore calculate



* Ratios requested in problem statement.

