#### Material and Energy Balances Prof.Vingesh Muthuvijayan Department of Biotechnology Indian Institute of Technology – Madras

#### Module No # 06 Lecture No # 28 – Part 1 Material Balance: A Review – Part 1

Hello everybody, welcome to today's lecture where we are going to review all the fundamentals that we learnt related to material balances still now. So let us start with this overall review which will give you a perfect clarity on whatever we have discussed. And finally we will perform an example problem which looks out all the fundamentals that we have covered and thereby giving you a full closure for what are material balance is and related problems.

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### General material balance equation

Law of conservation of mass

#### Input - Output + Generation - Consumption = Accumulation

- Types of material balances
  - Total balance
    - · Total mass of a system is always a constant
    - Mass can't be created or destroyed
      - Generation = 0; Consumption = 0
  - Component balance
    - · Individual components of the system
    - Generation = 0; Consumption = 0 for nonreactive species
- · Steady state is assumed



Let us first start with what is the general material balance equation? So material equation are based on law of conservation of mass so the equation itself is input – output + generation – consumption = accumulation. So using this general material balance equation we have performed calculations for various types of systems what are the types of material balances that we can write.

We can write a total mass balance total mass of a system is always concerned which means mass cannot be created or destroyed thereby the equation becomes input - output = accumulation because generation and consumption terms are 0 for the total balance. You can also write

component balances are written for the individual components that are present in the system here generation and consumption will be 0 for non-reactive species.

In most of our calculations we have been assuming steady state as I had already justified in the earlier lectures most chemical and bio chemical processes and industrial processes operate under steady state condition except for states are either a start up or shut down of the process. For this reason assuming steady state is a reasonable assumption and we can proceed with performing calculations by ignoring the accumulation term.

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### Choosing a basis

- If mass/amount/flow rate is given, use the given value
- If multiple values are given use them collectively
- If no values are given, assume a convenient basis
- · Convert all given values to one basis
  - Composition of solids and liquids  $\rightarrow$  mass fraction
  - Composition of gases  $\rightarrow$  mole fraction
  - Composition of Busco 2, and a second secon all values are either in masses or moles

The next major concept with respect to material balances is choosing a basis how do we choose an appropriate basis? If mass amount of flow rate I given in the problem then you use that as the basis for our calculation. If there are more than 1 mass of flow rates given then we use them collectively as the basis for our calculations if these values are not given then we will have to assume a convenient basis.

Using a convenient basis will make sure that calculations are simple we should also make sure that all the data given is converted to 1 basis. For example composition of solids and liquids is usually given in terms of mass fractions and mass percentages whereas composition of gases is given is terms of mole fractions. If such mixed units are given then I make sure that they are converted to the same basis so that calculations are simpler.

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## Mass balance vs Mole balance

- · For systems with reactions
  - Total mass is conserved
  - Total moles is **NOT** conserved
  - · Mass of individual components is conserved
  - · Moles of individual components is conserved
- Balances that can be written for systems with reactions
  - Total mass balance
  - · Component mass and mole balances

Then the next concept we should look at is what balance do we write do we write mass balance or a mole balance and for what system these would be valid. For system without reaction it does not matter both total mass and total moles are concerned mass of individual components and moles of individual components are also concerned. This is because there are no reaction happening and generation and conception terms are going to 0.

Balances which you can write the system without reaction would be total mass and total mole balance and similarly for component balances also you can write then in terms of masses and moles. However if you were to consider systems with reactions total mass is concerned but total moles of the system is not concerned in a reaction only mass will be concerned and the moles of the reactant the products are not the same.

However mass of individual component moles of individual components are concerned so we can write the following we can write the total mass balance and component mole and mass balances for system with reaction. When we write component mass and mole balances we need to understand that these reactive components will have generation and consumption term which have to be accounted for.

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### Points to remember: Single unit processes

- Splitter
  - · Composition of the feed and exit streams are the same
  - · Only one independent balance equation can be written
- Other processes
  - If the process has 'n' components, 'n' independent equations can be written
    - Total balance and (n 1) component balances
    - n component balances
- Filter
  - · Filtrate, the exit liquid is solid-free and contains the soluble components
  - Filter cake contains some accompanying liquid
  - Concentration of dissolved components in the filtrate and the liquid accompanying filter cake are same
  - Valid when the dissolved components are not absorbed by the filter cake other additives such as filter aids

When we talk about single unit processes what are the points we need to remember about some of the common single unit processes. For a splitter the composition of the feed and exit stream are the same which means only one independent balance equation can been written which is either the total mass balance or one of the component balances which would be simplified as the total mass balance.

For other processes if the process as N components then N independent equation can be written this could be one total mass balance and N -1 component balances or N component balances themselves. In case of a filter we need to understand that the filtrate is the exit liquid which is the solid free and contains the solvable component the filter cake is the solid which has some accompanying liquid.

We need to understand that the concentration of dissolved components in the filtrate and the liquid accompanying the filter cake are the same this is valid when the dissolve components are not absorbed by the filter cake or other additives which has filter aids which may be used during the filtration process.

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### Points to remember: Multiple-unit processes

- Most crucial step: Identifying the system to study
  - Most accurate way Start with the subsystem with zero degrees of freedom
  - Other efficient ways
    - Start with the overall system
    - Start with the first unit in the multiple-unit process
    - Start with the final unit in the multiple-unit process
- How do you choose which unit to start with?
  - Choose the system with the most information on flowrates and compositions of inlet and outlet streams
  - Make combinations of 2 or more subunits to define such a system
  - · Stream of interest should cross the system boundary



When we talk about multiple unit processes the important concept which we need to learn and master is to identify which system to start with. So most accurate way of choosing a system would be the enter process is to divide sub units and perform the degree of freedom analysis to identify which degree of 0 degree freedom and start calculation from there.

However this technique is extremely tedious and time consuming because of this there are more efficient and simpler way to start with the other efficient ways would be to first either start with the overall systems as a single system where we consider this as one unit itself or we first start with first sub unit of the system and start performing calculations or we can start with the final sub unit in the system and start performing the calculations.

Amongst this three where do we start? We usually choose a system where the most information is available for you. If there is a system where you have information about the flow rates and composition of the streams that are crossing the system boundary then that is that system you would want to start with the changes are that is the system which as 0 degree of freedom. If an single sub unit does not have such a system then you would make a system which basically a combination of two or more sub units.

The overall system which you would choose would be such a combination there if you have 0 degree of freedom that is where you want to start with. So when we perform these calculations another important aspect which we need to remember is if we have a stream of interest then that

particular has to cross the system boundary. By that what I mean is if you have to calculate the flow rate or composition of the particular stream then the system drawn should not encompass this particular stream.

This stream has to cross the system boundary either as input or as an output only when we do this we will be able to calculate the parameters for that particular stream another aspect which we need to remember is if we have no information about a stream we do not know either flow rate or the composition or both of them and it is not a stream of interest. It is not something we need to calculate then draw system in the way that this stream is encompassed by the systems so that we do not need to worry about calculating the flow rates of composition of something which we do not need.

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### Points to remember: Reactive processes

- Quantities that are conserved
  - Total mass
    - Generation = 0; Consumption = 0
  - Number of atoms of each element • Generation = 0; Consumption = 0
  - Mass and moles of individual components
    - Generation and consumption terms have to be calculated based on reaction stoichiometry
- Types of balances
  - Molecular species balances
  - · Atomic species balances



When we talk about reactive processes there are certain processors which we need to remember. What quantities are concerned for reactions mass is concerned total mass is concerned total mass cannot be created or destroyed which means generation and consumption term will be 0 when we write the total mass equation for a reactive process. When we talk about atoms for each of the elements the same law of conservation applies.

The number of atoms of each of the elements is concerned again here you would have generation and consumption terms going to 0. Mass and moles of individual components are also concerned generation and consumption terms have to be calculated for these particular components balances using the stoichiometric or other information that are available in the problem.

So basically you can write either molecular species balances or atomic species balances and amongst molecular species balances you would have generation and conception terms for the reactive species. And atomic species balances will not have generation or consumption terms another important thing we need to remember about atomic species balances is we are writing fo reach atom. For example if we have methane taking part in the reaction one mole of methane one molecule of methane would contain one atom of carbon and for atoms of hydrogen.

So even if you have one mole of methane coming into the reaction you would account for four moles of hydrogen atoms entering into the reaction. So this is important when we perform atomic species balances. Hydrogen balance for the example I just mentioned would be 4 times the number of moles of methane entering. So similar principles have to be applied for all the component are taking part in the reaction.

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Points to remember: Combustion reactions

- Reaction of a substance with oxygen to form CO<sub>2</sub>, CO, H<sub>2</sub>O, SO<sub>2</sub>, etc.
  - Complete combustion forms CO<sub>2</sub>, SO<sub>2</sub> and H<sub>2</sub>O
  - Partial combustion produces some CO
- Air is assumed to be 79%  $\rm N_2$  and 21%  $\rm O_2$  for ease of calculations
- N<sub>2</sub> is treated as non-reacting component by neglecting oxidation of N<sub>2</sub> to for NO<sub>x</sub>
- Remember the distinction between wet and dry basis



When we talk about combustion reactions what we need to remember is this is a reaction where the substance reacts with oxygen to form carbon dioxide carbon monoxide water vapor sulfur dioxide and so on. In complete combustion you would have carbon dioxide sulfur dioxide and water vapor being formed and in partial combustion you would have some amount of carbon monoxide also being formed. In most of the combustion reaction we can assume that air is 79% nitrogen and 21% oxygen for ease of calculations. So for such air the average molecular weight would be roughly 29 grams per mole. Nitrogen is treated as non-reacting component in combustion reaction and most reaction for that matter nitrogen forming knocks usually ignored while we preforming this calculations.

This is because this is usually very small and can be negligible therefore we can ignore it we need to remember the distinction between what is the wet basis and dry basis just as the refresher wet basis would account for the water vapor component present in the basis also whereas dry basis will not account for the water vapor present in the gases.

So if you have 10 moles of carbon di oxide 10 moles of water vapor and 10 moles of carbon monoxide in a flue gas then in dry basis carbon dioxide mole fraction would be 0.5 and carbon monoxide mole fraction would be 0.5. In wet basis carbon dioxide and carbon monoxide water vapor would all have mole fraction of 0.33 so this is what wet and dry basis are. When information is given we need to use them appropriately.

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### Points to remember: Biochemical reactions

- Michaelis-Menten equation mechanistic model for enzyme kinetics
- Monod's equation unstructured, nonsegregated model for growth kinetics
- Ideal CSTR/chemostat Reactor contents are well mixed
  - Concentration of all the components are the same in any part of the reactor
  - Concentration in the exit stream is the same as the concentration inside the reactor



When we come to biochemical reactions these are the following points we need to remember Michaelics Menton equation is a mechanistic model describing enzyme kinetics. You have Monod's equation as the instructed non segregated model for growth kinetics although we did nor describe or discussed how to derive Michaelics Menton equation I had mentioned earlier that it can be derived using the enzyme reaction that is why it is a mechanistic model.

Monod's equation cannot be derived it is more of an empirical model based on unstructured non segregated modeling which makes certain assumptions. So we talked about and ideal CSTR or Chemostat when we talk about bio chemical reactions these are re actor where the contents are well mixed. So what i mean by that is the concentration of all the components are same any part of the reactor. Concentration in the exit stream is the same as the concentration inside the reactor. **(Refer Slide Time: 13:28)** 

# Points to remember: Biochemical reactions

- Growth rate extensive property; specific growth rate – intensive property
- · Assumptions in Monod's model
  - · Cells can be represented as a single entity
  - · Cells are uniformly distributed in the culture
  - · A single substrate is growth-rate limiting



Other points about the biochemical reaction would involve what growth rate and specific growth rate are. Growth rate is an extensive property and specific growth rate is intensive property obtain from growth rate by dividing growth rate with the either the biomass concentration or the biomass number.

Assumption which are used in Monad's model are cells can be represented as single entity cells are uniformly distributed in the culture can cell sub state is growth rate is limited process.

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### Points to remember: Recycle, Bypass, & Purge

- At steady state, material circulates without accumulation
  Accumulation will be zero for any subsystem studied
- Recycle with reactions
  - Overall conversion
  - Single-pass ("once-through") conversion
- Bypass
  - Skips one or more stages and goes directly to another downstream stage
- Purge
  - Removed from the process to remove accumulation of inerts or unwanted material that might build up due to recycle



When we talk about recycle, bypass and purge there are certain concepts which we need to remember at steady state material circulation happens without accumulation during the recycle or bypass what I mean by this accumulation will be 0 for any sub system which is studying within the overall system recycle with reactions can have two types of conversions overall conversions and single pass conversion.

Overall conversion is basically the conversion which would happen for the overall system which includes the recycle stream whereas single pass conversion what happens when the reactants pass through the reactor only once by pass is a process where you have a streams skipping one or more of the stages to go directly into the downstream stage and purge is the process where some components are being removed so that you can avoid or accumulation of inerts are other unwanted materials which might build up due to recycle.

With this we have covered all the basis which we have talked about till now we will solve two example problems for getting the overall picture of whatever we discussed. The first example will talk about a chemical system where chemical reaction are taking place you would have a multi-unit system with recycle and purge. The second system which is the second example will talk about a bio chemical reaction. In today's lecture we will perform one example problem and the second example problem will be in a next lecture.