Chemical Reaction Engineering I
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Lecture 01
Introduction and Overview on Reaction Engineering

Welcome to the first introductory lecture on Chemical Reaction Engineering 1, as you know this course is divided into two part, one is chemical reaction engineering 1, where we will discuss mostly on homogeneous reactions and ideal and as well as non-ideal reactor designs and in the second part generally we consider the heterogeneous reactions, catalytic reactions and so on.

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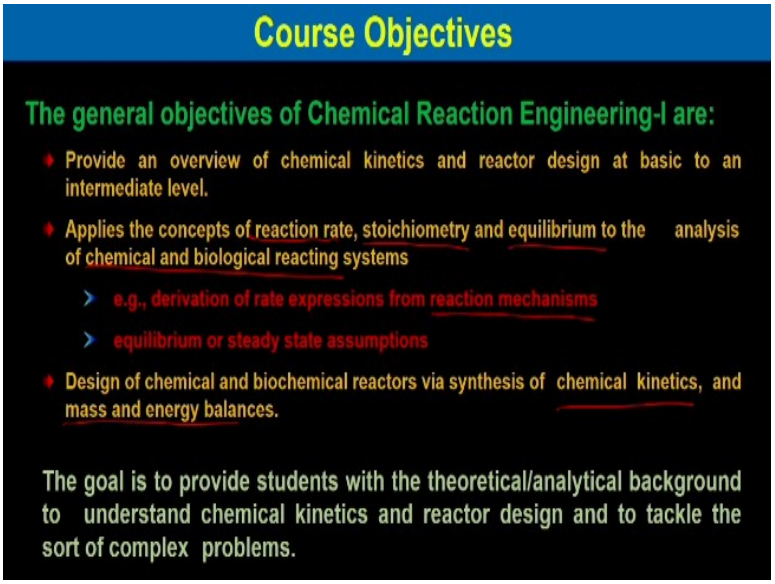

Course Objectives

The general objectives of Chemical Reaction Engineering-I are:

- Provide an overview of chemical kinetics and reactor design at basic to an intermediate level.
- Applies the concepts of reaction rate, stoichiometry and equilibrium to the analysis of chemical and biological reacting systems
  - e.g., derivation of rate expressions from reaction mechanisms
  - equilibrium or steady state assumptions
- Design of chemical and biochemical reactors via synthesis of chemical kinetics, and mass and energy balances.

The goal is to provide students with the theoretical/analytical background to understand chemical kinetics and reactor design and to tackle the sort of complex problems.

So, our course is mostly on the first part, before going to this lecture, let us have our objectives of this course. The general objectives of chemical reaction engineering 1 are to provide an overview of chemical kinetics and reactor design at basic to the intermediate level and this course will apply the concept of reaction rate, then stoichiometry and equilibrium to the analysis of different chemicals and biological reacting systems.

For example, derivation of rate expression from the reaction mechanism or we can take the concept from the equilibrium or steady state assumptions for certain reactions. So, design of Chemical and Biochemical reactors via synthesis of chemical kinetics and mass and energy balances. So, this course will also consider the design of reactors, which will take into account the chemical kinetics as well as mass and energy balances wherever necessary.

The broad goal of this course is to provide students with theoretical and analytical background so that they can understand the chemical kinetics and the reactor design to tackle the sort of complex problem.

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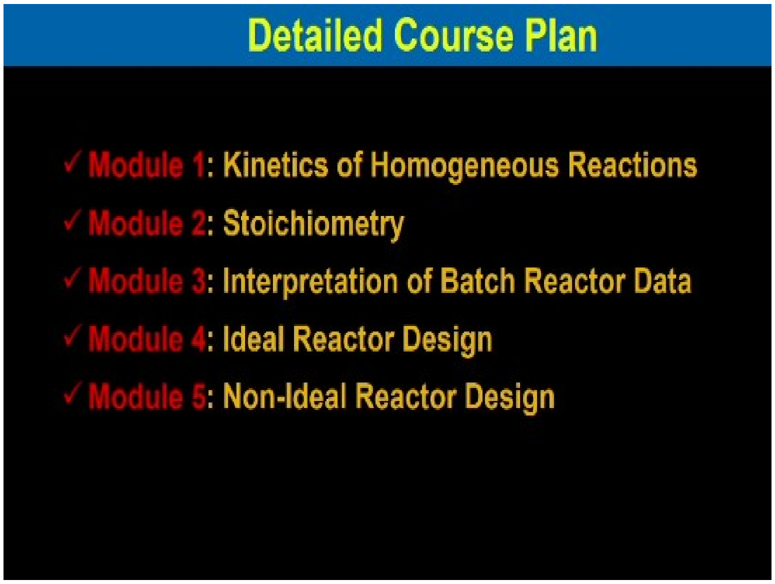

Detailed Course Plan

- ✓ Module 1: Kinetics of Homogeneous Reactions
- ✓ Module 2: Stoichiometry
- ✓ Module 3: Interpretation of Batch Reactor Data
- ✓ Module 4: Ideal Reactor Design
- ✓ Module 5: Non-Ideal Reactor Design

The detailed course plan for this in module 1 we will consider the kinetics of homogeneous reactions. And in Module 2 we will consider stoichiometry, module 3 we will discuss interpretation of the batch reactor data and in module 4 we will consider ideal reactor design and module 5 non ideal reactor design. So these five modules we will consider most of our topic to be covered in this course.

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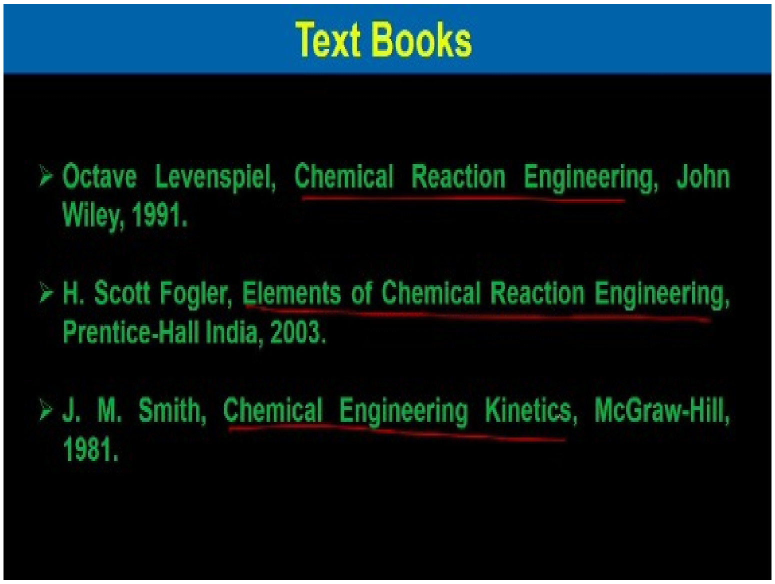

Text Books

- Octave Levenspiel, Chemical Reaction Engineering, John Wiley, 1991.
- H. Scott Fogler, Elements of Chemical Reaction Engineering, Prentice-Hall India, 2003.
- J. M. Smith, Chemical Engineering Kinetics, McGraw-Hill, 1981.

The textbooks which we generally follow for chemical reaction engineering 1. The first one is Octave Levenspeil, that is on chemical reaction engineering. The second book is H. Scott Fogler, that is elements of chemical reaction engineering and the third one is James Smith, chemical engineering kinetics. In addition to that, we will have many reference books which we will highlight while we discuss different topics in this lecture series.

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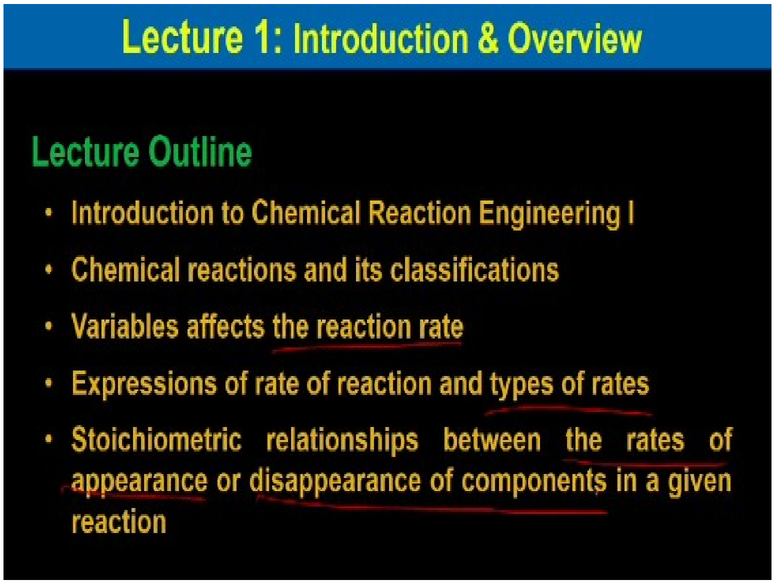

Lecture 1: Introduction & Overview

Lecture Outline

- Introduction to Chemical Reaction Engineering I
- Chemical reactions and its classifications
- Variables affects the reaction rate
- Expressions of rate of reaction and types of rates
- Stoichiometric relationships between the rates of appearance or disappearance of components in a given reaction

So, the brief introduction and overview of this course will be covered in this lecture. The lecture outline would be introduction to chemical reaction engineering, then we will consider chemical reactions and its classification, the different variables which affect the reaction rate, then how to express the rate of reaction and their different types of rates, then Stoichiometric relationship between the rates of appearance of particular component and disappearance of a particular components in a given reaction, so those things we will consider.

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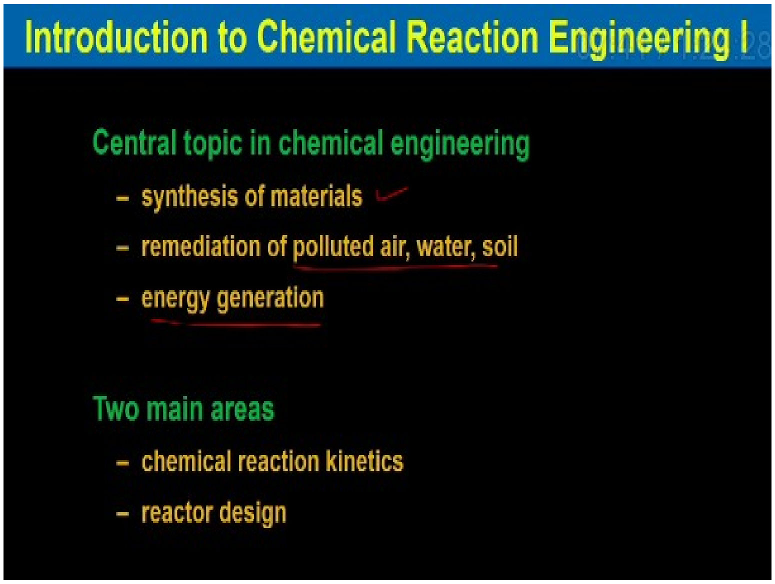

Introduction to Chemical Reaction Engineering I

Central topic in chemical engineering

- synthesis of materials
- remediation of polluted air, water, soil
- energy generation

Two main areas

- chemical reaction kinetics
- reactor design

Before going to this lecture, let us understand what are the central topic for chemical engineers. There are three important topic for chemical engineers to understand, one is synthesis of materials, as you know in day to day life we use different materials like our clothes, paste and starting from all the materials we use every day, they are finished products, but it has produced through a succession of steps. So, from raw material to product, chemical engineers has great roles on producing the finished products.

The second thing is the remediation of the polluted air, water and soil. As you know, our air, water and soil are polluted day by day due to different human activities and industrialization. If we consider air pollutions as you know today, the greenhouse effect the major pollutants, which create the greenhouse effect is the carbon dioxide we use to hear every day in our newspaper and on so on and we are experiencing a drastic climate change, water pollutions as you know, although on the earth, there are plenty of water major part is the water but the drinking water or the water which to be utilized are very scarce. So, it gets polluted because of different industrial processes and we have to make it clean by different means and similar to the soil pollution.

So, remediation of polluted air, water and soil is an another important topic for the chemical engineers to work with. And third is the energy generation, energy as you know, this is the one important thing which we need for everything to run, without energy we cannot survive. So, we need to have enough quantum of energy to be produced, so that it meets all the industrial and other requirements.

The two main areas we will consider in chemical reaction engineering, one is chemical kinetics and the other one is reactor design. So, in first part of this lecture in this module, we will consider the chemical reaction kinetics and later part we will consider the reactor design part.

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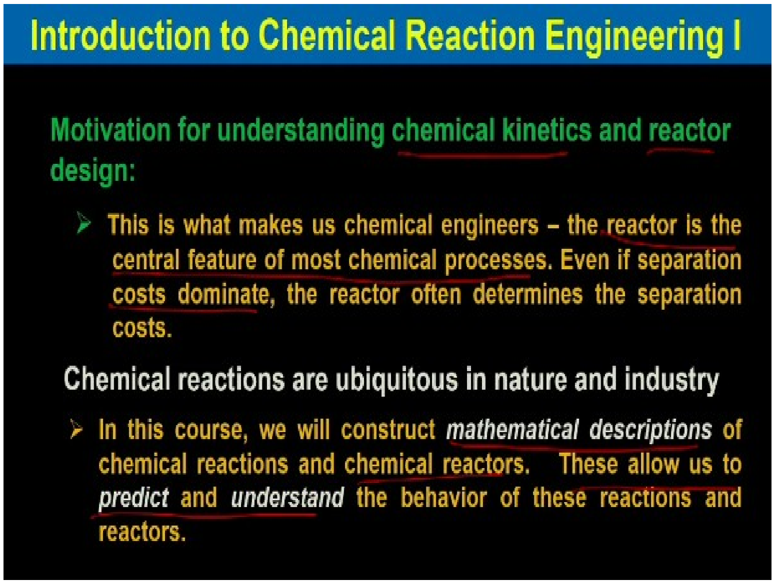

Introduction to Chemical Reaction Engineering I

Motivation for understanding chemical kinetics and reactor design:

- This is what makes us chemical engineers – the reactor is the central feature of most chemical processes. Even if separation costs dominate, the reactor often determines the separation costs.

Chemical reactions are ubiquitous in nature and industry

- In this course, we will construct *mathematical descriptions* of chemical reactions and chemical reactors. These allow us to *predict* and *understand* the behavior of these reactions and reactors.

So, motivation for understanding chemical kinetics and reactor design because as you know this only thing, only subjects which distinguish between the chemical engineers to the other engineers as we know, reactor is the central features for most of the chemical processes, and even if the separation cost dominates the reactor often determines the separation cost.

If the reactor is efficient and produce product which are of high purity, then its separation may not be required after the product is formed. So, the separation cost in that case would be minimum, but if the reactor is not efficient enough so that the product which you will produce have to be separated and that separation cost might be much higher compared to the overall reactor cost, so inevitably this chemical reactors are the central feature for any chemical industries.

Chemical reactions are ubiquitous in nature and in industry as you know. So this course will construct the mathematical description of chemical reactions and chemical reactors. So, it will represents the chemical reactions and chemical reactors in mathematical form which we call the design equations or the modeling of rate or rate of reactions or the reactor design or modeling of reactors.

So, we will construct the mathematical description that means the physical system is represented in a mathematical form and this will allow us to predict and understand the view here of different reactions and reactors.

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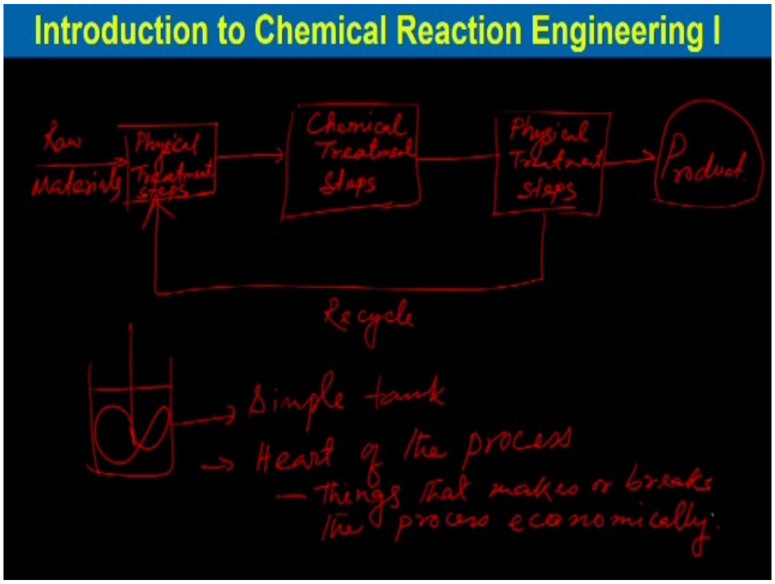
Introduction to Chemical Reaction Engineering I

Every chemical industrial processes is designed to produce economically desired product from different starting materials. Let us take an example suppose, if you have the raw materials and these raw materials may not be fed to the chemical reactor, it needs some physical separations, so it should go physical treatment steps, then once it goes via the physical treatment steps, it will be fed to the chemical reactors, so chemical treatment steps.

Once the chemical treatment is done or it is fed to the chemical reactors the reactions would take place and it will produce the products, the product may not be pure, so the products which we will produce that again will go to several physical treatment steps and then you will get the product. So, once physical treatment steps is followed over here, the raw material which is not converted is again fed to the physical treatment steps, so, that it is again fed to the chemical treatments, so this is recycle. So this physical treatment steps means once the product is produced that has to be separated or some purification has to be done so that we can get the finished products.

The physical treatments steps will not be covered over here, because this is already covered in your mechanical operation course, or the unit operation course, where most of the physical treatment steps have been considered like you have seen in your mechanical operation course, the different physical separations which we used to do in our labs. One is the different types of crusher where you take ores from the industry's big chunk of ores and then you crash into different small fractions that is jaw crusher, roll crusher and different types of crusher.

Again you can also reduce the size in a ball mill or hammer mill and then you can separate them by different other physical separation steps like you can have screening of the materials or you can have froth flotation, cyclone separation, so many other physicals separation steps, so that will not be covered over here. So, here we will mostly consider on chemical treatment steps.

In chemical treatments steps, it may be a simple reactor or simple tank, simple mixing tank, but although it is simple, but this is what makes or breaks the process economically. So, although it looks simple, but this is the heart of the process, that means this economically makes or breaks the process, so design of chemical reactors is not a routine matter there are many alternatives, maybe available for a reactor design.

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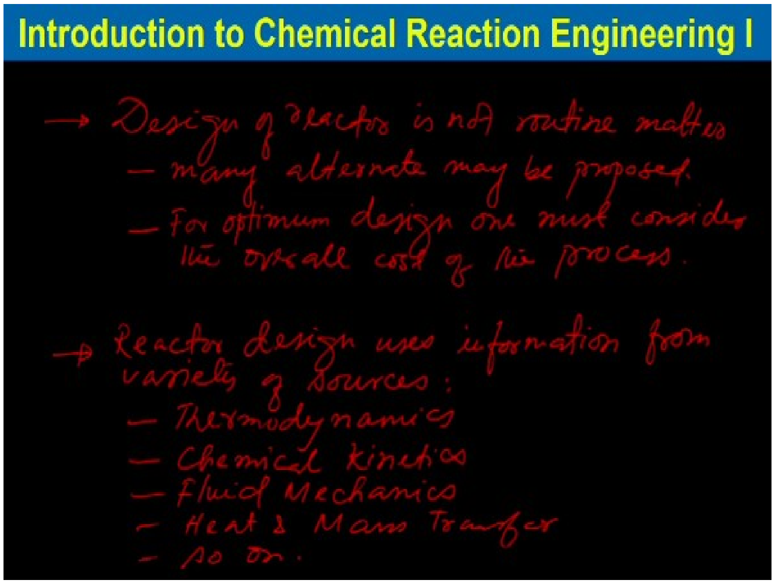

Introduction to Chemical Reaction Engineering I

→ Design of reactor is not routine matter
  - many alternate may be proposed.
  - For optimum design one must consider the overall cost of the process.

→ Reactor design uses information from variety of sources:
  - Thermodynamics
  - Chemical kinetics
  - Fluid Mechanics
  - Heat & Mass Transfer
  - so on.

So, in searching of the reactor design, one must have to optimize for the cost. So, in one design may be superior with respect to the other design so the cost of the overall process have to be considered while designing a chemical reactors. So design of reactor is not routine matter, many alternate may be proposed. For optimum design one must consider the overall cost of the process. Reactor design you just the information from variety of sources, like thermodynamics it also uses the chemical kinetics, fluid mechanics, heat and mass transfer and so on.

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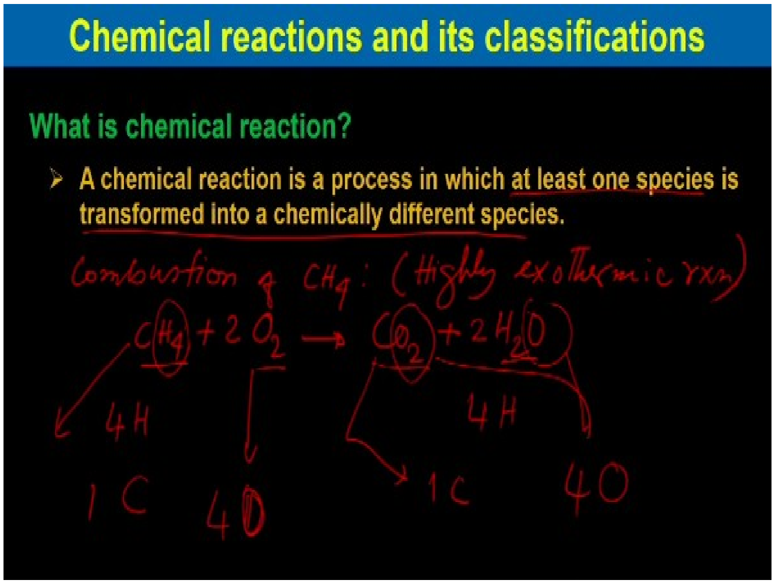

Chemical reactions and its classifications

What is chemical reaction?

- A chemical reaction is a process in which at least one species is transformed into a chemically different species.

Combustion of CH_4: (Highly exothermic rxn)

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Let us start with what is chemical reaction? A chemical reaction is a process in which at least one species is transformed into chemically different species. Let us consider combustion of methane, this is a very highly exothermic reaction methane react with oxygen and it forms carbon dioxide and water vapor.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2 0$$

So in this reactions as you can see the reactants is methane and oxygen and it produce the different compound that is carbon dioxide and water, but as you could see the number or type of molecules may change, that means, you can see that the total type of molecules earlier we had methane and oxygen, which is converted to carbon dioxide and water vapor. So, the type of molecules have changed after the chemical reactions.

However, their constituents or the building block materials remains the same that means before the reactions the reactants had 4 methane so, the hydrogen 4H and after the reactions you could see also 4H, before reactions we had one carbon and after the reactions we have one carbon, before the reactions we had 4 oxygen atom and after the reactions we have 2 and 2 over here, so 4O. So that means the elements or the building block materials that remain same before the chemical reactions, but after the chemical reactions, but the molecular or the number of molecules or the species have changed before the reaction and after the reaction.

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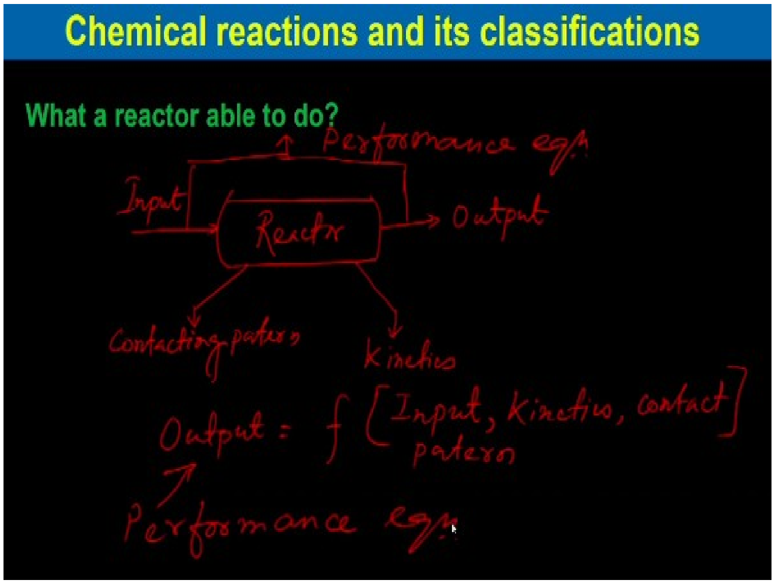

Chemical reactions and its classifications

What a reactor able to do?

Now, to find out what a chemical reactor able to do, let us consider a chemical reactor and you have input to the reactor and you have output and in between inside this is your reactor and you need to know the contacting pattern inside the reactor, that means the reactant materials when it is fed to the reactor, how they contact, how they flow inside the reactor, whether they are well mixed with each other or whether they are segregated from each other, how they flow what is the contacting pattern inside the reactor?

Similarly, we should also know the kinetics of the reactions, whether the reaction is very fast or if it is very fast then the equilibrium will tell us what the product will produce. Similarly, if the reaction is very slow then the chemical kinetics or the rate of reactions will tell us what would be the chemical kinetics for that reactions. So all these informations we need to know when a raw material is processed inside a reactor to obtain output and we have to find out the relations between the input and the output.

So the equations which would relate between the input and output is known as the Performance Equation, so we can write output is a function of input, kinetics and contact pattern and this is known as Performance Equation.

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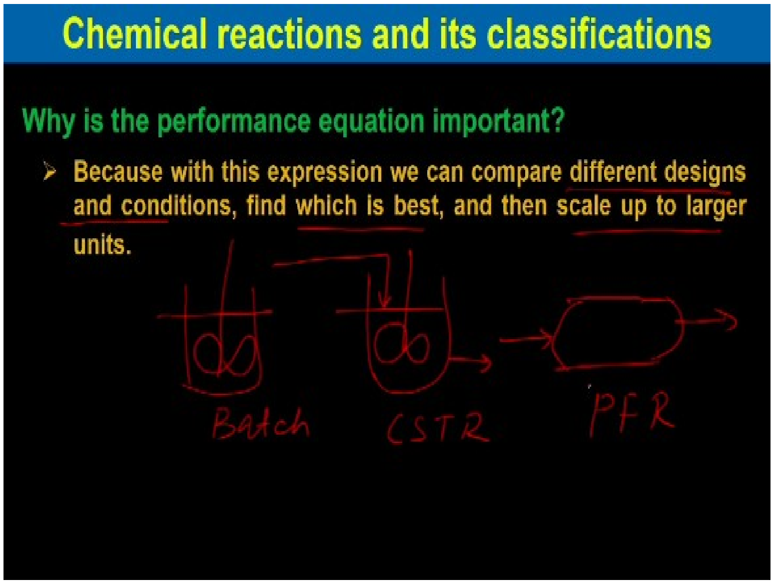

Chemical reactions and its classifications

Why is the performance equation important?

- Because with this expression we can compare different designs and conditions, find which is best, and then scale up to larger units.

Now, why this Performance Equation is important? Because this is the expression we can compare different designs and conditions and from that we can find out which is the best one and then scale up to the larger units, while discussing we will consider three idealized reactors, let us introduce very little bit, you have batch reactor like this where you dump the material and stir it there is no input and output we call batch reactor.

Then you have flow reactors, one of them CSTR where you (feed) fed the material, stir it and there is a constant output from the reactors, this is called continuous stir tank reactor, this is CSTR, this is batch and another idealized reactor is the plug flow reactor, we will discuss more about the idealized reactor later, plug flow reactor and from the Performance Equation or for a particular reaction to happen we can and under the different conditions we can compare these three reactor design, which one would be best among them and then how to scale up that to the larger unit, that we can discuss or we can get from the Performance Equation and that is why it is very important to design a reactor based on the mathematical description of that reactors, which is the Performance Equation.

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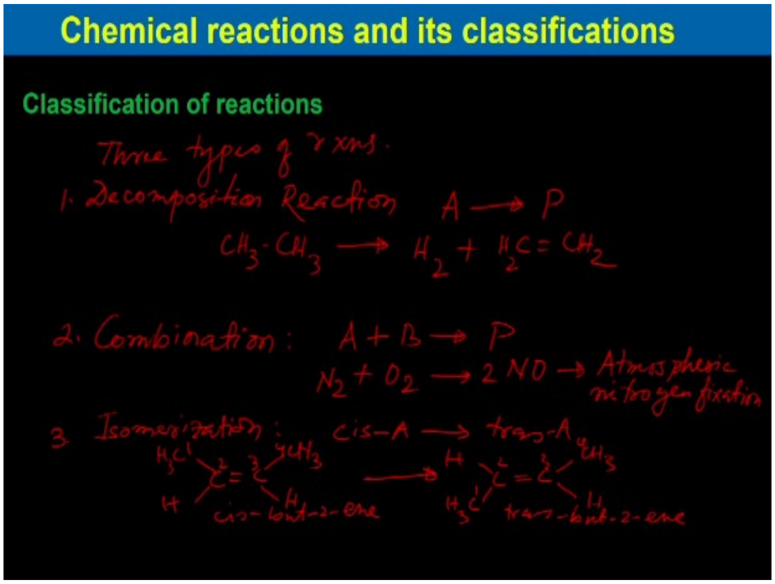

Chemical reactions and its classifications

Classification of reactions

Three types of rxns.

1. Decomposition Reaction $A \rightarrow P$

$CH_3-CH_3 \rightarrow H_2 + H_2C=CH_2$

2. Combination: $A + B \rightarrow P$

$N_2 + O_2 \rightarrow 2NO \rightarrow$ Atmospheric nitrogen fixation

3. Isomerization: cis-A $\rightarrow$ trans-A

Now, classifications of reactions, there are many ways we can classify chemical reactions, the one general type of classification is there are three types of reactions, one is decomposition reaction, that means a reactant would be converted to product, so reactant A decomposes to produce product P. For example, if we consider ethane CH_3-CH_3 and it decomposes to hydrogen and ethylene, so this is one of the example of decomposition reaction.

The second reaction is combination reaction. For example, if we take reactant

$$A + B \rightarrow P$$

so A combined with B produces product P. For example, if we consider nitrogen react with oxygen produced nitric oxide. So, this is one of the example of combination reactions as you know, this is one of the famous examples of atmospheric nitrogen fixation reactions.

The nitrogen in the atmosphere during heavy lightning, it reacts with oxygen at high temperature and produce nitric oxide and then it converted to nitric oxide and the nitric oxide again falls with water and forms nitric acid which again calcium carbonate reacts with nitric acid forms calcium nitrate and then it is converted to different usable form of for the plants. So, this is one of the famous example of atmospheric nitrogen fixation.

The third type of reactions is the isomerization reaction that means our compound say cis A forming to trans A, so cis-trans isomerization of a particular compound, like if we consider cis butene C double bond C and CH_3,H cis means the methane same group on the same site. So this is cis but-2-ene and this converted to trans so here this is 1, 2, 3 and 4, so this converted to C double bonds CCH_3HHCH_3 so 1, 2, 3, 4 so this is trans but-2-ene, so most of the chemical reactions are can be clubbed into these three types of reactions.

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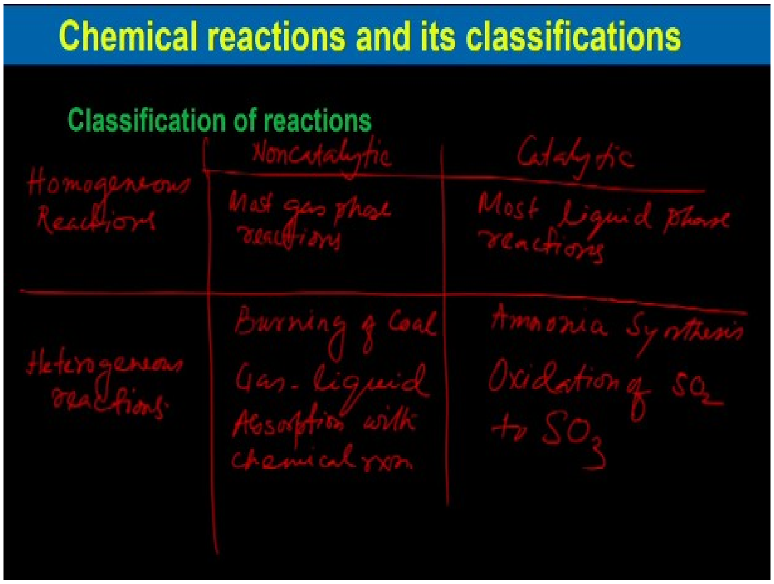

Chemical reactions and its classifications

Classification of reactions

	Noncatalytic	Catalytic
Homogeneous Reactions	Most gas phase reactions	Most liquid phase reactions
Heterogeneous reactions	Burning of Coal Gas-liquid Absorption with chemical rxn	Ammonia Synthesis Oxidation of SO_2 to SO_3

In chemical reaction engineering the best way to classify the chemical reactions is to how many phases are involved for the chemical reactions. So, in view of these the chemical reactions are classified into two categories, one is homogeneous reactions that is the reactions takes place in one phase and the other one is the heterogeneous reaction.

So, homogeneous reaction and then the second one is the heterogeneous reaction. The homogeneous reactions can also be catalytic or non-catalytic process, so we can again distinguish both the processes catalytic and non-catalytic, most gas phase reactions are non-catalytic in nature and most liquid phase reactions are catalytic in nature under homogeneous reaction conditions.

The heterogeneous reactions, for example, under non catalytic is burning of coal, as you know for the energy generation most of the power plants they uses coal as a main source of their energy productions. So they burn coal and produce energy and it generates huge amount of carbon dioxide released to the atmosphere.

So gas liquid absorption with chemical reaction here in the catalytic process is ammonia synthesis, oxidation of sulfur dioxide to sulfur trioxide as you can see all these are required two phases in case of burning of coal it is solid and gas, then gas liquid is a gas and liquid two phases. So, these are non-catalytic process and these are the catalytic process, Haber's process for ammonia synthesis is one of the very important example of catalytic heterogeneous reactions.

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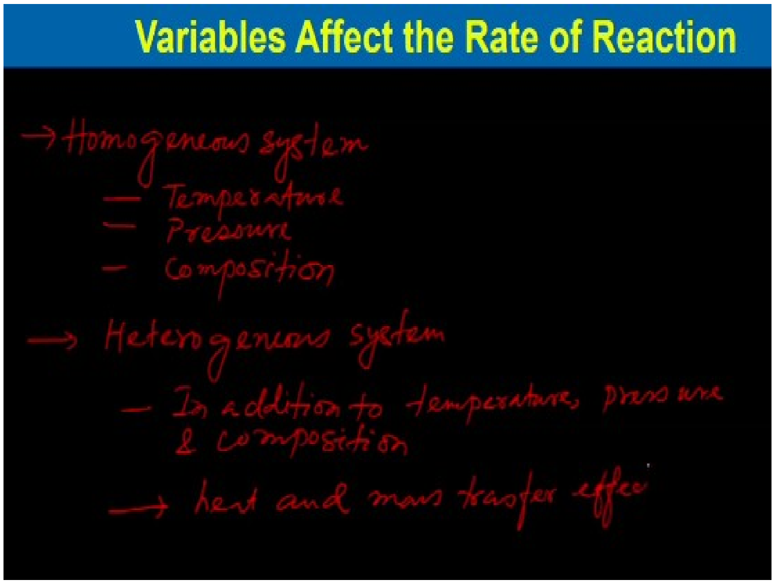

Variables Affect the Rate of Reaction

→ Homogeneous system
- Temperature
- Pressure
- Composition

→ Heterogeneous system
- In addition to temperature, pressure & composition

→ heat and mass trasfer effec

Different variables which affects the rate of chemical reactions, as we have classified the reactions into two categories based on the number of phases involved, one is homogeneous reactions and another is heterogeneous reactions, if the homogeneous reactions that is reactions takes place in single phase then the variables which would affect the rate of chemical reactions are temperature, pressure and composition.

So, for homogeneous system the variables are temperature, pressure and composition or concentration, for heterogeneous system that is more than two phases involve, it becomes more complex because, when we consider say gas solid heterogeneous reactions the particles are porous, the reactions take place on the solid surface of the different catalyst materials, so the solute molecules or the reactants has to travel through the solute to the catalyst particles to react on the active sites. So this depending on the pores and the structure of the catalyst, it creates different mass transfer limitations.

In addition to that, suppose, the reactions is taking place on the catalyst surface or inside the porous structure of the catalyst, the heat generated if it is very exothermic process the heat which would generate due to the chemical reactions, how fast this would release or this would transport to the outer surface it depends on the structure of the catalyst.

So it also (influence) affects the rate of chemical reactions, so in addition to the parameters which affects the heterogeneous system it also affects including those parameters it also required the heat transfer effect and the mass transfer effect in case of the heterogeneous reaction. So in case of heterogeneous reaction in addition to temperature, pressure and composition we need to consider heat and mass transfer effects.

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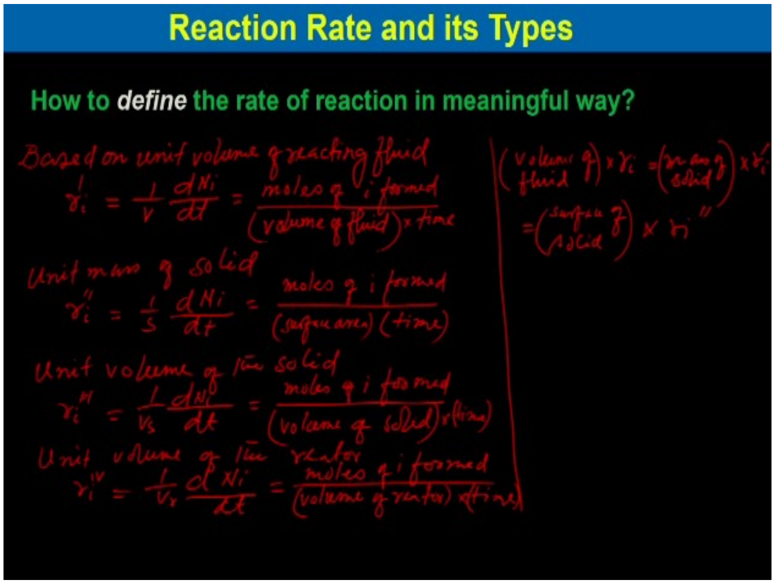

Reaction Rate and its Types

How to *define* the rate of reaction in meaningful way?

Based on unit volume of reacting fluid

$$r_i' = \frac{1}{V}\frac{dN_i}{dt} = \frac{\text{moles of } i \text{ formed}}{(\text{volume of fluid}) \times \text{time}}$$

Unit mass of solid

$$r_i'' = \frac{1}{S}\frac{dN_i}{dt} = \frac{\text{moles of } i \text{ formed}}{(\text{surface area})(\text{time})}$$

Unit volume of the solid

$$r_i''' = \frac{1}{V_s}\frac{dN_i}{dt} = \frac{\text{moles of } i \text{ formed}}{(\text{volume of solid}) \times (\text{time})}$$

Unit volume of the reactor

$$r_i^{iv} = \frac{1}{V_r}\frac{dN_i}{dt} = \frac{\text{moles of } i \text{ formed}}{(\text{volume of reactor}) \times (\text{time})}$$

$$\begin{pmatrix}\text{volume of}\\ \text{fluid}\end{pmatrix} \times r_i = \begin{pmatrix}\text{mass of}\\ \text{solid}\end{pmatrix} \times r_i' = \begin{pmatrix}\text{surface of}\\ \text{solid}\end{pmatrix} \times r_i''$$

So, how to define the rate of reactions in meaningful way? So to answer these questions let us have different definitions of rate of reaction, one is based on unit volume of reacting fluid that is r_i is the rate of reaction is equal to $\frac{1}{V}\frac{dN_i}{dt}$ that is moles of I formed divided by volume of fluid into time, if it is the reactions which is happening in the solid phase then we can define based on unit mass of the solid in the fluid solid systems.

So based on unit mass of solid we can write r_i is equal to $\frac{1}{S}\frac{dN_i}{dt}$ which is equal to moles of I formed divided by surface area into time, we can also define based on volume of the solids, unit volume of the solid, so we can write rate is equal to $\frac{1}{V_S}$ that is volume of solid $\frac{dN_i}{dt}$, so which is the moles of I formed divided by volume of solid into time. We can also define in terms of the volume of the reactor, so we can also write in terms of the volume of the reactor, so where we can define

$$r_i = \frac{1}{V_r}\frac{dN_i}{dt}$$

which is equal to moles of I formed divided by volume of reactor into time.

So these definitions you will get in the know chapter 1 of Levenspiel book and just I am highlighting over here. So these are different rates and we can relate among them like volume of fluid into r_i would be mass of solid into $r_i^{'}$ which would be equal to surface of solid into $r_i^{''}$ and so on. So, this way we can define the rate of reactions.

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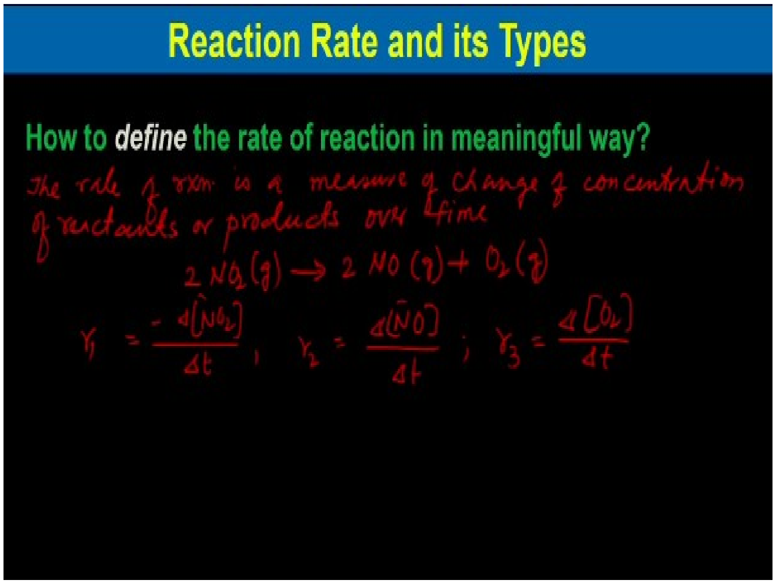

Reaction Rate and its Types

How to *define* the rate of reaction in meaningful way?

The rate of rxn is a measure of change of concentration of reactants or products over time

$2NO_2(g) \rightarrow 2NO(g) + O_2(g)$

$r_1 = \frac{-\Delta[NO_2]}{\Delta t}, \quad r_2 = \frac{\Delta[NO]}{\Delta t}; \quad r_3 = \frac{\Delta[O_2]}{\Delta t}$

The rate of reaction is a measure of change of concentration of reactants or products over time. So we can define the rate of reaction is a measure of change of concentration of reactants or products over time, suppose if you consider the reaction

$$2NO_2(\mathrm{g}) \rightarrow 2\,\mathrm{NO(g)} + O_2(\mathrm{g})$$

We can write various rates

$$r_1 = -\frac{\Delta[NO_2]}{\Delta t}$$

Similarly, we can write

$$r_2 = \frac{\Delta[NO]}{\Delta t}$$

or we can write

$$r_3 = \frac{\Delta[O_2]}{\Delta t}$$

and we can relate these three rate stoichiometrically,

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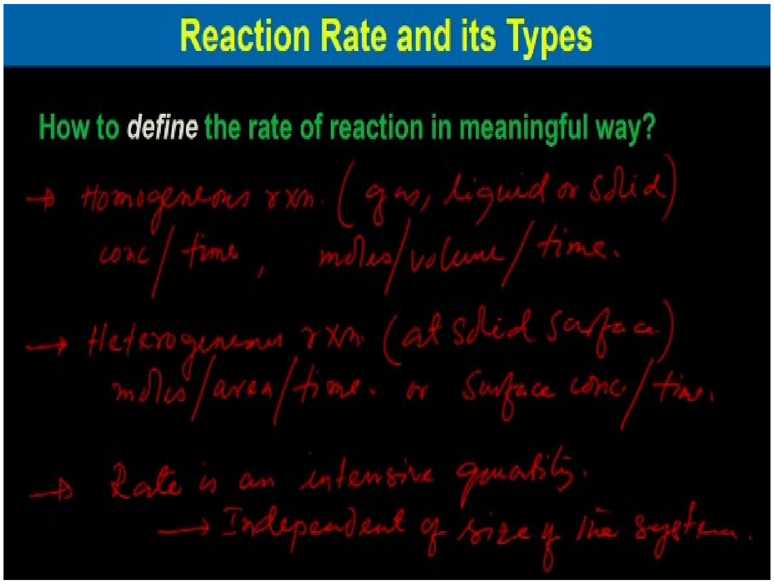

Reaction Rate and its Types

How to *define* the rate of reaction in meaningful way?

→ Homogeneous rxn. (gas, liquid or solid)
conc/time, moles/volume/time.

→ Heterogeneous rxn (at solid surface)
moles/area/time. or Surface conc/time.

→ Rate is an intensive quantity.
→ Independent of size of the system.

For homogeneous reaction that means the gas, liquid or solid whatever may be the phase the rate units or the concentration, concentration per time or moles per volume per time, if it is heterogeneous reaction then that is at solid surface in that case we can define moles per area per time or surface concentration per time, this rate is an intrinsic property rate is an intensive quantity, intensive quantity that means the dependence of the rate is not there with respect to the size of the reactors that is the reaction rate is independent of size of the system, sometimes also we refer to extensive rates that means, the intensive rate is multiplied by the volume of the reactor.

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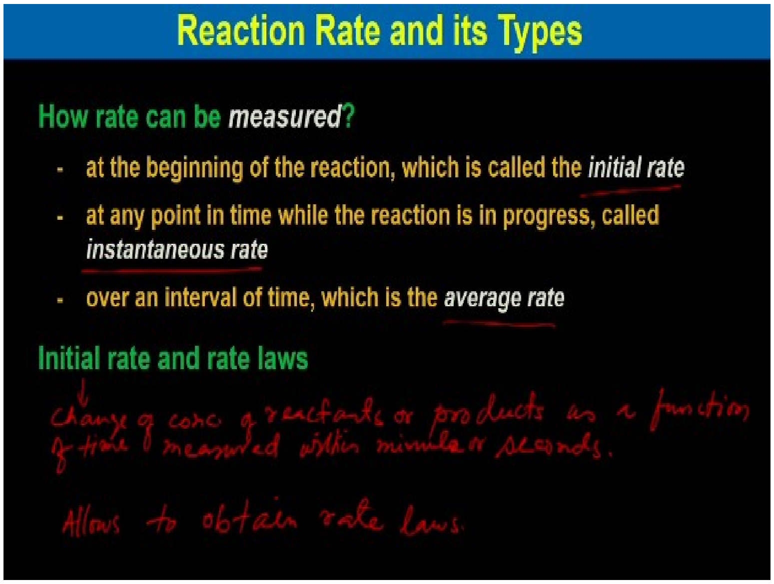

Reaction Rate and its Types

How rate can be *measured*?

- at the beginning of the reaction, which is called the *initial rate*
- at any point in time while the reaction is in progress, called *instantaneous rate*
- over an interval of time, which is the *average rate*

Initial rate and rate laws

Change of conc. of reactants or products as a function of time measured within minutes or seconds.

Allows to obtain rate laws.

How rate can be measure? So we can measure the rate at three different ways, one that is at the beginning of the reactions that is which is called the initial rate. Secondly, we can also measure the rate of reaction at any point of time of the chemical reactions to progress, so we call it instantaneous rate. And then the third way we can do over an interval of time where we calculate the average rate.

Initial rate and rate laws, initial rate means the rate of change of concentration of reactant product in the initial, very initial stage maybe in first minute or few seconds, that is that initial rates when the reaction starts. So initial rate is basically the change of concentration of reactants or products as a function of time measured within minutes or seconds.

So these initial rates allows us to determine the rate laws and rate law is the mathematical representation of the dependency of the reaction rate with the change of concentration, so at a particular temperature, so this initial rate allows us to obtain rate laws.

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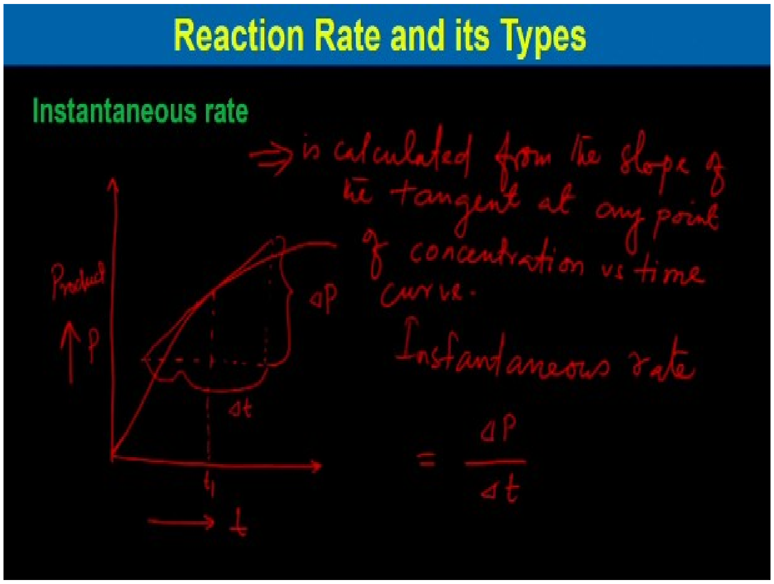

Reaction Rate and its Types

Instantaneous rate

⇒ is calculated from the slope of the tangent at any point of concentration vs time curve.

Instantaneous rate $= \frac{\Delta P}{\Delta t}$

Now, let us consider instantaneous rate, the instantaneous rate can be calculated from the temperature concentration, from the concentration time plot that means the variation of concentration with respect to time plot and if we plot a tangent at any point on the concentration time curve from the slope of that tangent we can calculate the instantaneous rate.

Suppose, this is your product concentration and this is time, is like this, so we can plot a tangent at any point say at time t_1 the slope of this curve can be obtained this means this is your ΔP, if this is product P and this would be Δt that is time. So the instantaneous rate would be equal to $\frac{\Delta P}{\Delta t}$ that means the rate is calculated from the slope of the tangent at any point of concentration versus time curve, so this is the instantaneous rate.

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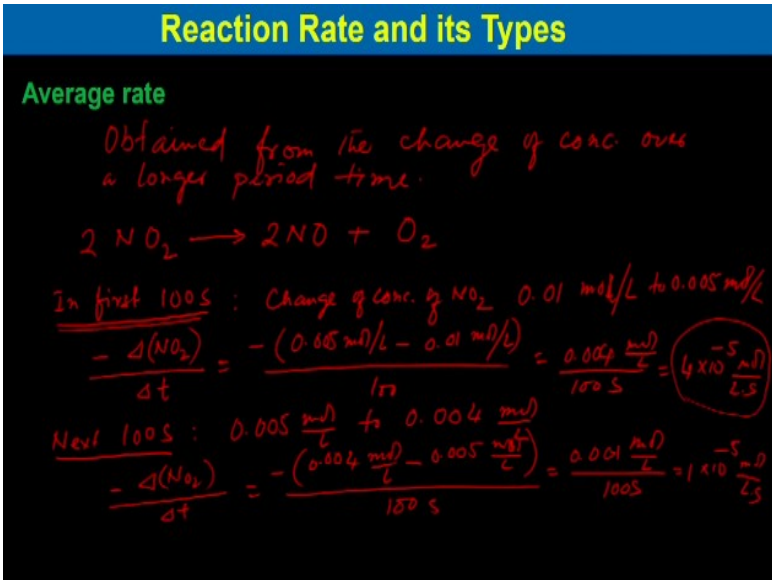

Reaction Rate and its Types

Average rate

Obtained from the change of conc. over a longer period time.

$2NO_2 \longrightarrow 2NO + O_2$

In first 100 s : Change of conc. of NO_2 0.01 mol/L to 0.005 mol/L

$-\frac{\Delta(NO_2)}{\Delta t} = \frac{-(0.005\,mol/L - 0.01\,mol/L)}{100} = \frac{0.004\,\frac{mol}{L}}{100\,s} = \boxed{4\times10^{-5}\,\frac{mol}{L\,s}}$

Next 100 s : 0.005 $\frac{mol}{L}$ to 0.004 $\frac{mol}{L}$

$-\frac{\Delta(NO_2)}{\Delta t} = \frac{-\left(0.004\,\frac{mol}{L} - 0.005\,\frac{mol}{L}\right)}{100\,s} = \frac{0.001\,\frac{mol}{L}}{100s} = 1\times10^{-5}\,\frac{mol}{L\,s}$

Now, let us consider the average rate. Average rate is obtained from the change of concentration over a longer period of time. So this is obtained from the change of concentration over a longer period of time. Now, let us consider an example suppose the reaction of nitrogen dioxide that is

$$2NO_2 \rightarrow 2\,\mathrm{NO} + O_2$$

and the change of concentration was observed in first 100 seconds say the change of concentration of NO_2 it happens from 0.01 mole per liter to 0.005 mole per liter.

So if this is the change for the first 100 second, then we can calculate $-\frac{\Delta[NO_2]}{\Delta t}$ would be equal to minus 0.005 mole per liter minus 0.01 mole per liter divided by 100, so it is 0.004 mole per liter divided by 100 seconds. So it would be $4*10^{-5}$ mole per liter second.

Now, in the next 100 second, the change of concentration is from 0.005 mole per liter to 0.004 mole per liter. So, this is the change of concentration in the next 100 seconds. So then we can calculate minus $\frac{\Delta[NO_2]}{\Delta t}$ would be equal to minus 0.004 mole per liter minus

0.005 mole per liter divided by 100 second. So this should be equal to 0.001 mole per liter divided by 100 second.

So this will give $1*10^{-5}$ into 10 to the power minus 5 mole per liter second. So as you can see the change of concentration when the concentration of nitrogen dioxide was more the rate of change becomes more that means about 4 times higher compared to the next 100 seconds this happens because the concentration of the reactant drops over the time.

So the average rate will obviously be much less compared to the initial rate because the instantaneous rate is gradually changing, because of our gradually decreasing because of change in concentration.

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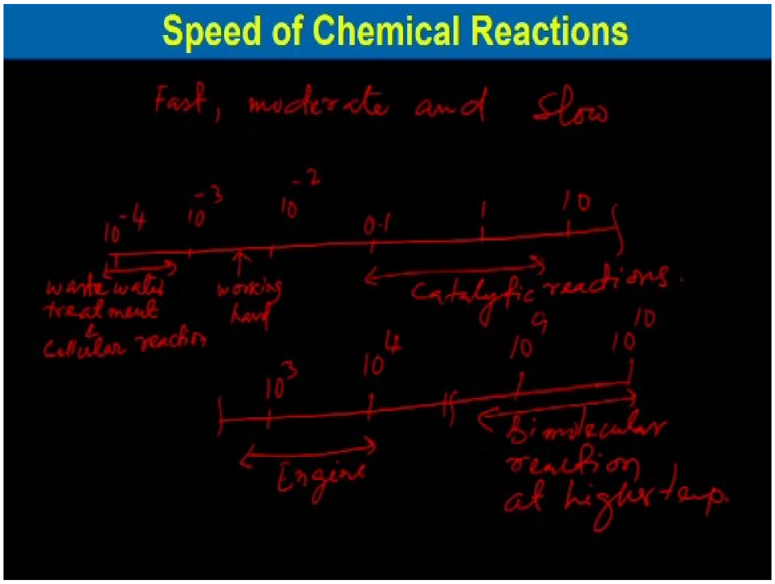

Speed of Chemical Reactions

Fast, moderate and slow

Now, let us look into the speed of chemical reaction, as you know there are some reactions which occurs very fast, like if you consider the reactions of petroleum production, that is production of the gasoline from crude oil or we can consider the productions of plastics that is the polyethylene production the reaction is very very fast. Whereas, in some reactions like biological reactions or wastewater degradation or treatment of wastewater that takes quite longer time for the reactions to happen, very slow reactions.

So, if we look into the overall scheme, so as we said the fast reactions and slow reactions and in between you have moderate reactions, fast, moderate and slow. So to look into this let us see how the reactions can happen for what systems have higher reaction rates and which system has lower reaction rates.

So different order of the reactions that is the speed of the chemical reactions are shown with respect to 10 to the power some exponents. If we look into the reaction rate in case of the cellular reactions or wastewater treatment systems. So, wastewater treatment and cellular reactions those are in the order of 10^{-4} to 10^{-3} in this order. If we look in the human working human systems, when they are working conditions, they are in the order of close to 10^{-2}, for catalytic reactions, they are in this range.

Now, if you consider the reactions of different engines like jet engines and rocket engines those are very fast, those are in the order of 10^{3} to 10^{4}, so they are in these high speed reaction region and some of the bimolecular reactions or gas phase reactions at higher temperature the reactions happens to be very very fast which is in the order of 10 to the power 9 to 10 to the 10 so in this rage. So this shows the rate of chemical reactions which occurs at different systems.

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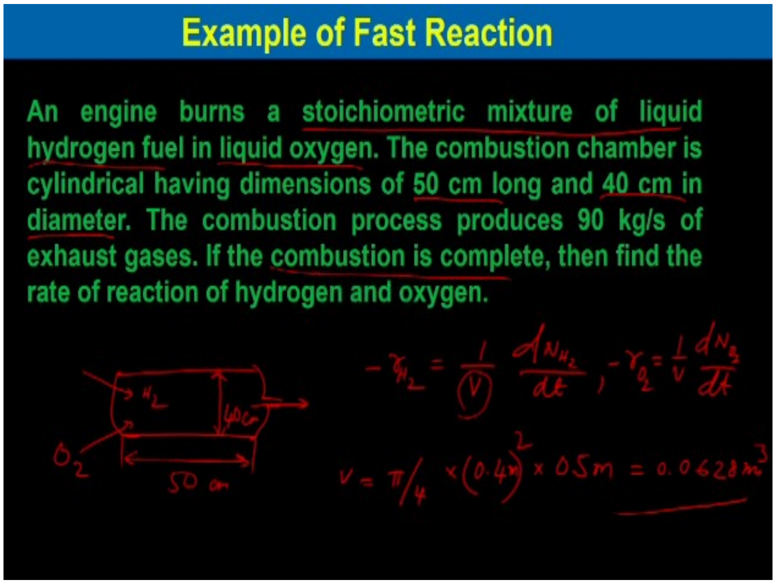

Example of Fast Reaction

An engine burns a stoichiometric mixture of liquid hydrogen fuel in liquid oxygen. The combustion chamber is cylindrical having dimensions of 50 cm long and 40 cm in diameter. The combustion process produces 90 kg/s of exhaust gases. If the combustion is complete, then find the rate of reaction of hydrogen and oxygen.

$$-r_{H_2} = \frac{1}{\boxed{V}}\frac{dN_{H_2}}{dt}, \quad -r_{O_2} = \frac{1}{V}\frac{dN_{O_2}}{dt}$$

$$V = \pi/4 \times (0.4m)^2 \times 05m = 0.0628 m^3$$

Now, let us consider an examples where the rate of reactions is very fast. So, an engine burns a stoichiometric mixture of liquid, that is liquid fuel hydrogen and liquid oxygen and it happens in the combustion chamber and then the chamber is cylindrical dimensions that is 50 centimeter long and 40 centimeter diameter. The combustion process produces 90 kg per second of exhaust gas and we need to find out the rate of reactions of hydrogen and oxygen and it is assumed that the combustion process is complete.

So as per the problem given so we can just look draw the combustion engine or combustion chamber where we have, so where product is coming out after the combustion, so we have hydrogen, we have oxygen inside and its length is 50 centimeter and this dia is 40 centimeter. And as per the problem given we need to find out minus RH to the rate of reactions of hydrogen which reacts with oxygen and produce the water vapor. So this is the rate of reactions would be

$$-r_{H_2} = \frac{1}{V}\frac{dN_{H_2}}{dt} \text{ and } -r_{O_2} = \frac{1}{V}\frac{dN_{O_2}}{dt}$$

So, these two you need to calculate.

So, let us calculate the volume, so the volume for these combustion chamber is equal to pi by 4 into D square, D is 0.4 meter so into L is 0.5 meter. So this will give around 0.0628 meter cube so this is the volume of the combustion chamber.

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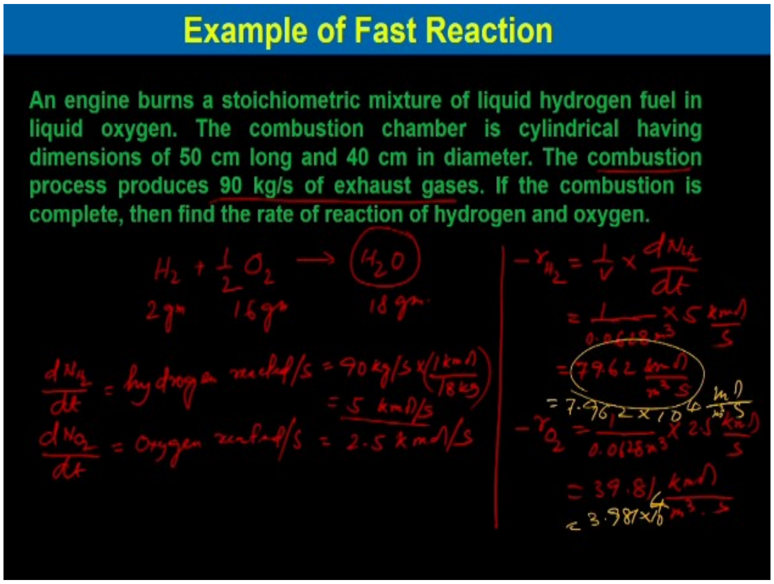

Example of Fast Reaction

An engine burns a stoichiometric mixture of liquid hydrogen fuel in liquid oxygen. The combustion chamber is cylindrical having dimensions of 50 cm long and 40 cm in diameter. The combustion process produces 90 kg/s of exhaust gases. If the combustion is complete, then find the rate of reaction of hydrogen and oxygen.

$H_2 + \frac{1}{2}O_2 \rightarrow \boxed{H_2O}$

2 gm 16 gm 18 gm

$\frac{dN_{H_2}}{dt}$ = hydrogen reacted/s = 90 kg/s × $\left(\frac{1\ kmol}{18\ kg}\right)$ = 5 kmol/s

$\frac{dN_{O_2}}{dt}$ = Oxygen reacted/s = 2.5 kmol/s

$-r_{H_2} = \frac{1}{V} \times \frac{dN_{H_2}}{dt}$

$= \frac{1}{0.0628\ m^3} \times 5 \frac{kmol}{s}$

$= 79.62 \frac{kmol}{m^3 s}$

$= 7.962 \times 10^4 \frac{mol}{m^3 s}$

$-r_{O_2} = \frac{1}{0.0628\ m^3} \times 2.5 \frac{kmol}{s}$

$= 39.81 \frac{kmol}{m^3 . s}$

$\approx 3.981 \times 10^4$

Now, let us look into the reactions which is happening. The reactions between hydrogen plus oxygen forming H_2O. Now, if we write the balanced equation hydrogen half oxygen will produce H2O. Now, the molecular weight of this is 2 gram, this is 16 gram and this is 18 gram. So we can calculate the $\frac{dN_{H_2}}{dt}$ that is the hydrogen produced per second which is equal to 90 kg per second into 1 kilomole by 18 kg. So which is equal to 5 kilomole per second that means the combustion process produces 90 kg of the exhaust gas, so our exhaust gas is water vapor.

So its molecular weight is 18, so we can calculate as we can see, 1 mole of hydrogen can produce 1 mole of water vapor for this combustion reactions. So hydrogen production rate would be 5 kilomole per second whereas, from the stoichiometry if we look into that half oxygen produced 1 mole of H_2O. So $\frac{dN_{O_2}}{dt}$ would be the oxygen, hydrogen reacted per second would be 2.5 kilomole per second.

So then we can calculate the reaction rate of hydrogen $-r_{H_2}$ would be equal to $\frac{1}{V}\frac{dN_{H_2}}{dt}$ if we put the values of the volume that is 1 by 0.0628 meter cube into 5 K mole per second. So this would be 79.62 kilomole per meter cube second.

Similarly, we can obtained the r_{O_2} would be just half of this rate of reactions of hydrogen, so it would be 1 by 0.0628 meter cube into 2.5 kilo mole per second. So this should give 39.81 kilomole per meter cube second. So, if we write this in terms of the mole per meter cube second, so this would be equal to $7.962*10^4$ mole per meter cube second, and this would be $3.981*10^4$. So as we can see the order of the this the reaction rate is of the order of 10^4, this is the fast reaction.

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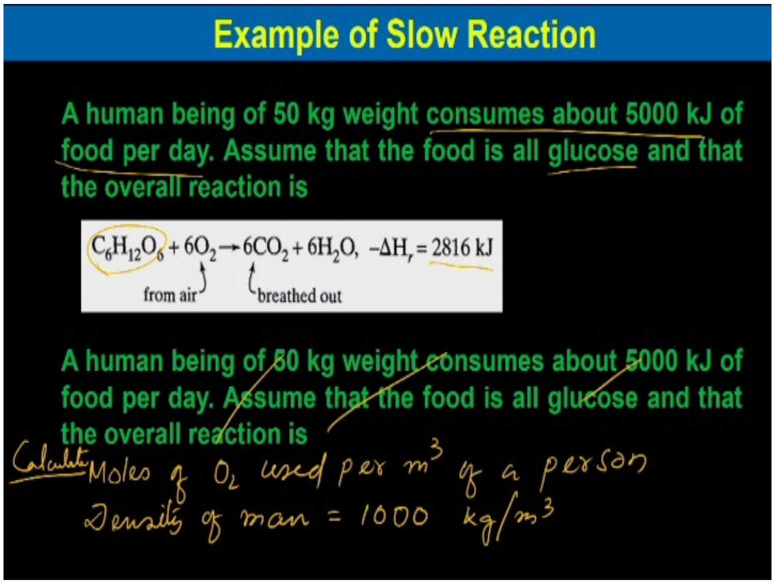

Example of Slow Reaction

A human being of 50 kg weight consumes about 5000 kJ of food per day. Assume that the food is all glucose and that the overall reaction is

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O, \quad -\Delta H_r = 2816 \text{ kJ}$$

from air

breathed out

A human being of 50 kg weight consumes about 5000 kJ of food per day. Assume that the food is all glucose and that the overall reaction is

Calculate Moles of O_2 used per m^3 of a person

Density of man = 1000 kg/m^3

Now, let us take another example of slow reaction. A human being of 50 kg weight consumes about 5000 Kilo Joule of food per day and assume that the food is glucose and that the overall reactions is represented by this that means glucose reacts with oxygen and produce carbon dioxide and water and it is exothermic reactions. So it releases the heat ΔH twice 2816 kilo Joule.

So, if this is the case then we need to find out moles of oxygen used per meter cube of a person given the density of man is equal 1000 KG per meter cube. So we need to calculate moles of oxygen used per meter cube of a person having density of man is 1000 kg per meter cube.

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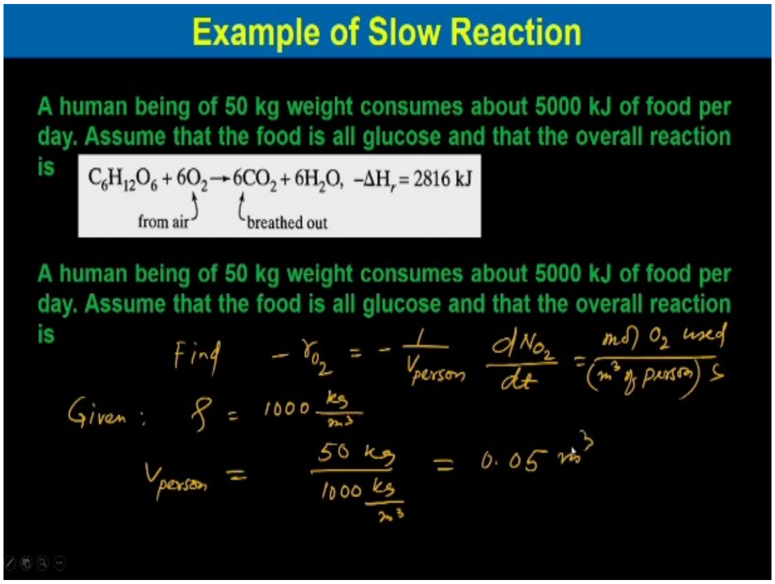

Example of Slow Reaction

A human being of 50 kg weight consumes about 5000 kJ of food per day. Assume that the food is all glucose and that the overall reaction is

$$C_6H_{12}O_6 + \underset{\text{from air}}{6O_2} \rightarrow \underset{\text{breathed out}}{6CO_2} + 6H_2O, \quad -\Delta H_r = 2816 \text{ kJ}$$

A human being of 50 kg weight consumes about 5000 kJ of food per day. Assume that the food is all glucose and that the overall reaction is

Find $-r_{O_2} = -\frac{1}{V_{person}}\frac{dN_{O_2}}{dt} = \frac{\text{mol } O_2 \text{ used}}{(m^3 \text{ of person})\, s}$

Given : $\rho = 1000 \frac{kg}{m^3}$

$$V_{person} = \frac{50 \text{ kg}}{1000 \frac{kg}{m^3}} = 0.05 \text{ m}^3$$

So, what we need to find out? r_{O_2} is equal to $-\frac{1}{V}\frac{dN_{O_2}}{dt}$ that is mole oxygen used per meter cube of person per second, this we need to calculate. Given that density is 1000 Kg per meter cube. So the volume of the person we can calculate weight of the person that is 50 kg divided by the density 1000 kg per meter cube which is 0.05 meter cube.

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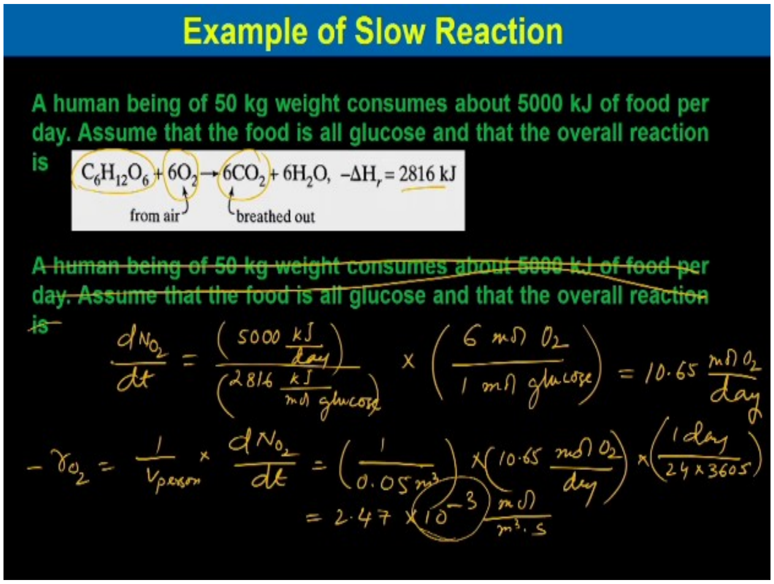

Example of Slow Reaction

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$$\underset{}{C_6H_{12}O_6} + \underset{\text{from air}}{6O_2} \rightarrow \underset{\text{breathed out}}{6CO_2} + 6H_2O, \quad -\Delta H_r = 2816\ \text{kJ}$$

~~A human being of 50 kg weight consumes about 5000 kJ of food per day. Assume that the food is all~~ glucose and that the overall reaction ~~is~~

$$\frac{dN_{O_2}}{dt} = \frac{\left(5000\ \frac{kJ}{day}\right)}{\left(2816\ \frac{kJ}{mol\ glucose}\right)} \times \left(\frac{6\ mol\ O_2}{1\ mol\ glucose}\right) = 10.65\ \frac{mol\ O_2}{day}$$

$$-r_{O_2} = \frac{1}{V_{person}} \times \frac{dN_{O_2}}{dt} = \left(\frac{1}{0.05\ m^3}\right) \times \left(10.65\ \frac{mol\ O_2}{day}\right) \times \left(\frac{1\ day}{24 \times 3605}\right)$$

$$= 2.47 \times 10^{-3}\ \frac{mol}{m^3 . s}$$

Now, as we can see the each mole of glucose reacting with 6 mole of oxygen and producing 6 mole of carbon dioxide and 6 mole of water and releasing energy which is 2816 kilo Joule. So now, let us calculate $\frac{dN_{O_2}}{dt}$ would be equal to 5000 kilo Joule per day into divided by 2816 kilo Joule per mole glucose into 6 mole of oxygen by 1 mole glucose.

So this will give about 10.65 mole of oxygen per day. Now, if we include this in the equations that is

$$-r_{O_2} = \frac{1}{V}\frac{dN_{O_2}}{dt}$$

we obtain 0.1 by 0.05 meter cube into 10.65 mole oxygen per day. So this would essentially give, now, if we just convert day to second, so this would be 1 day divided by 24 into 360 seconds. So this would be about $2.47 * 10^{-3}$ mole per meter cube second.

So, you could see that the rate of reactions is in the order of 10^{-3}. So this is the slow reactions example of slow reactions which is happening in the human consumptions of the food in human being. So these examples shows us that the slow and fast reactions and reactions happen in the different speed. So thank you for hearing this lecture and we will continue our discussion in the next lecture.