Lecture #1.2

Chemical Reaction Engineering (CHE331A, 9 credits) Pre-req ESO201A

- Course Policy
- Course content

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Goals of Chemical Reaction Engineering

- Design Reactors by studying the rate and mechanisms of chemical reactions
- Conduct Chemical Reactions at controlled conditions to:
  - Maximize selectivity (multiple products: D and U)
  - Maximize yield (get the most out of the conversion)
  - Maximize energy efficiency
  - Minimize impact to the environment
- Develop quantitative understanding of the reaction
- Selecting appropriate reactions and executing them in a controlled fashion

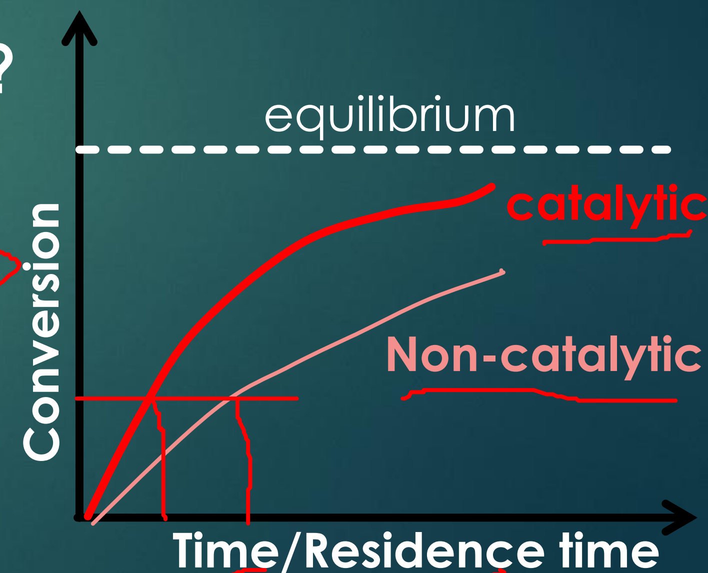
A chemical reaction has occurred!

- Molecules of one or more species have lost their identity and are present in a new form
  - Change in kind or number of atoms in the compound, and/or
  - Change in structure or configuration of these atoms

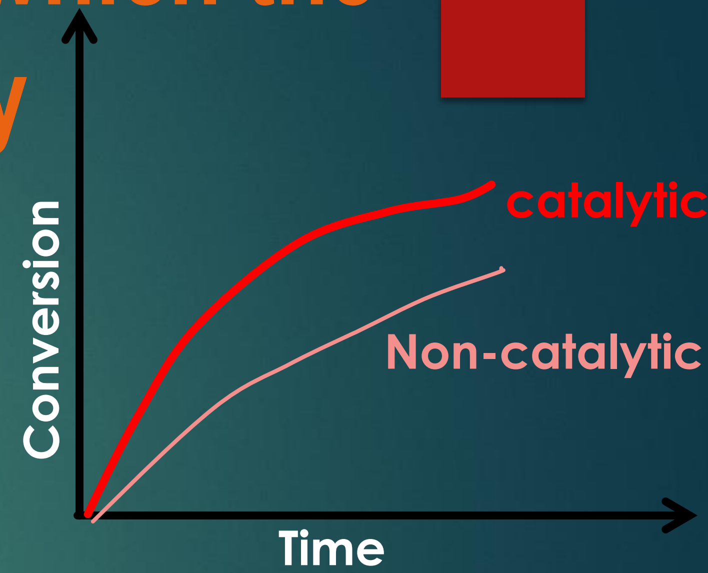
- Three basic ways a species may lose its identity
  - Decomposition $H_3C\text{-}CH_3 \rightarrow H\text{-}H + H_2C{=}CH_2$
  - Combination $N_2 + O_2 \rightarrow 2NO$
  - Isomerization $C_2H_5CH{=}CH_2 \rightarrow H_2C{=}C(CH_3)_2$

“Chemical Engineering” Thermodynamics set the stage

- **aA + bB → cC + dD** **Why did A react with B?**
  - Think thermo → ΔG
- **What is the extent of reaction?**
  - Think equilibrium → extent of reaction
- **Was there any heat evolved or required?**
  - Think energies → Q, W and ΔH
- **How quickly did they react?**
  - Think rate → time required conversion



Reaction rate is the rate at which the species looses their identity



- Reaction rate (rate) is expressed as:
  - Rate of formation
  - Rate of disappearance
  - Net rate (Multiple reactions)
  - Typical units are: $\dfrac{mol}{dm^3.s}$, $\dfrac{mol}{g-cat.s}$, or $\dfrac{mol}{m^2.s}$

- For example A → P (isomerization)
  - r_A is the rate of formation of A
  - $-r_A$ is the rate of disappearance of A
  - r_P is the rate of formation of P, $r_P = -r_A$

In general, r_j, is the rate of formation of species 'j'

r_j is

- a function of temp, press, conc and type of catalyst (if used)
- Independent of the type of Reactor used
- An algebraic equation, e.g., $r_j = -k.C_i C_j^2$
  - Other forms of the equation are possible
- Not a differential equation, e.g., rate is not $\frac{dC_A}{dt}$

$\frac{dC_A}{dt} = -r_A$ used to calculate the rate for certain conditions