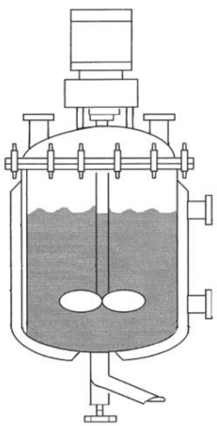
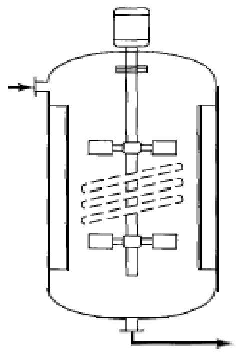
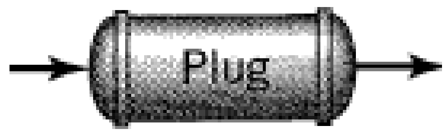
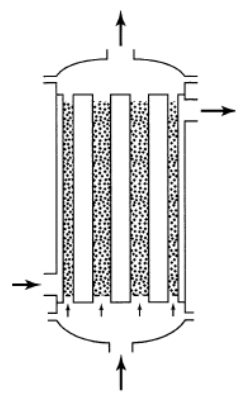
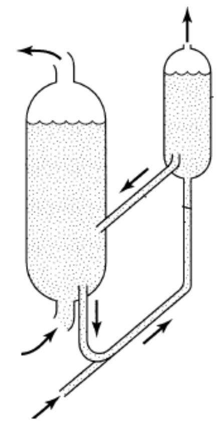
CHEMICAL REACTION ENGINEERING

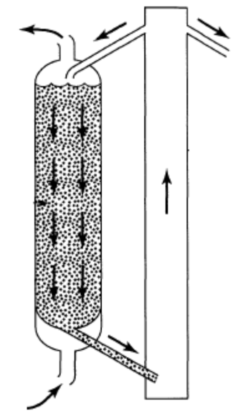












A. SARATH BABU

Course No. Ch.E – 326 CHEMICAL REACTION ENGINEERING

Periods/ Week : 4		***Credits: 4***
Examination	*Teacher Assessment:*	*Marks: 20*
	Sessionals: 2 Hrs	*Marks: 30*
	End Semester: 3 Hrs	*Marks : 50*

1. KINETICS OF HOMOGENEOUS REACTIONS
2. CONVERSION AND REACTOR SIZING
3. ANALYSIS OF RATE DATA
4. ISOTHERMAL REACTOR DESIGN
5. CATALYSIS AND CATALYTIC RECTORS
6. ADIABATIC TUBULAR REACTOR DESIGN
7. NON-IDEAL REACTORS

TEXT BOOKS

1. Elements of Chemical Reaction Engineering - Scott Fogler H
2. Chemical Reaction Engineering - Octave Levenspiel
3. Introduction to Chemical Reaction Engineering & Kinetics, Ronald W. Missen, Charles A. Mims, Bradley A. Saville
4. Fundamentals of Chemical Reaction Engineering – Charles D. Holland, Rayford G. Anthony
5. Chemical Reactor Analysis – R. E. Hays
6. Chemical Reactor Design and operation – K. R. Westerterp, Van Swaaij and A. A. C. M. Beenackers
7. The Engineering of Chemical Reactions – Lanny D. Schmidt
8. An Introduction to Chemical Engineering Kinetics and Reactor Design – Charles G. Hill, Jr.
9. Chemical Reactor Design, Optimization and Scaleup – E. Bruce Nauman
10. Reaction Kinetics and Reactor Design – John B. Butt

Without chemical reaction our world would be a barren planet. No life of any sort would exist.

There would be no fire for warmth and cooking, no iron and steel to make even the crudest implements, no synthetic fibers for clothing, and no engines to power our vehicles.

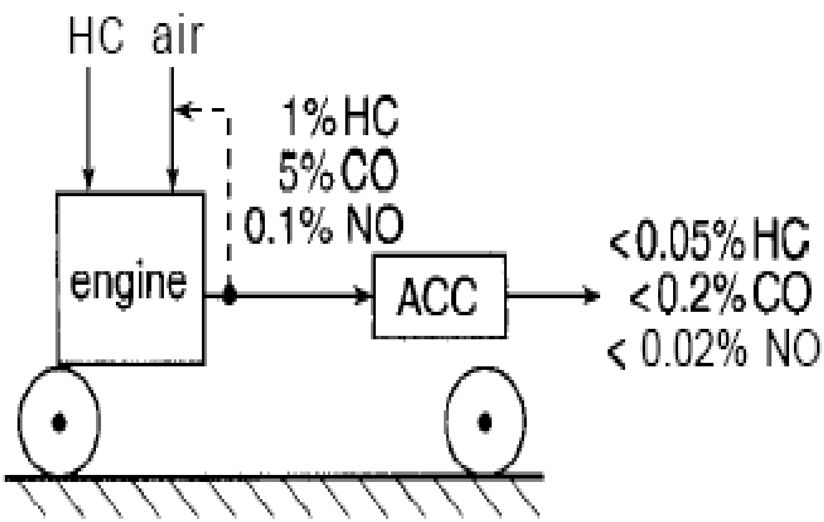
One feature that distinguishes the chemical engineer from others is the ability to analyze systems in which chemical reactions occur and to apply the results of the analysis in a manner that benefits society.

Automotive catalytic converter

The largest market for chemical reactors is the automotive catalytic converter (ACC), both in number of reactors in existence (many million sold/year) and in amount of reactants processed (millions of tons/year).

There are >50 million automotive catalytic converters operating throughout the world, and everyone owns one if he or she has a car less than 10 years old.

The catalytic converter is a tube wall reactor in which a noble-metal impregnated wash coat on an extruded ceramic monolith creates surface on which reactions occur.

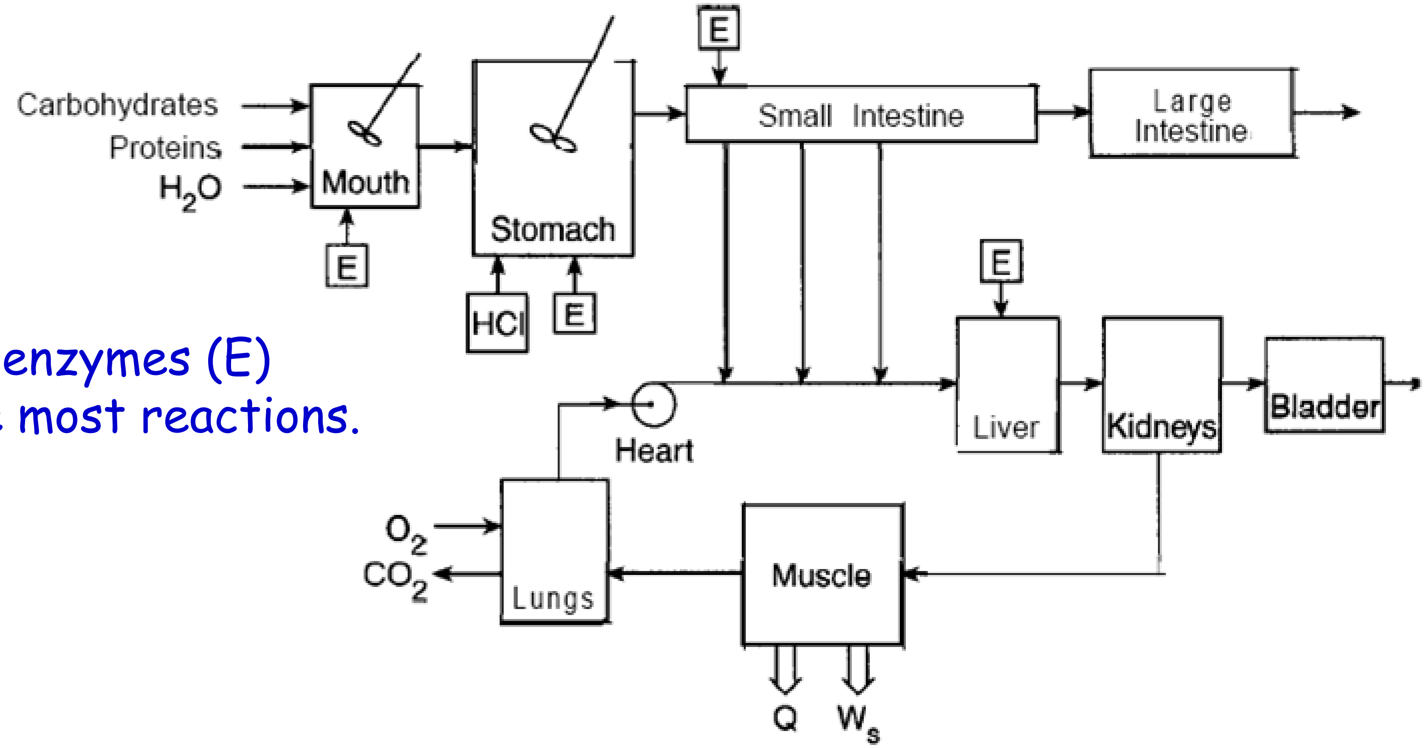


FCC Reactor

The FCC reactor is without question the most complex and important equipment in chemical engineering.

It is only second to ACC in amount of reactants processed.

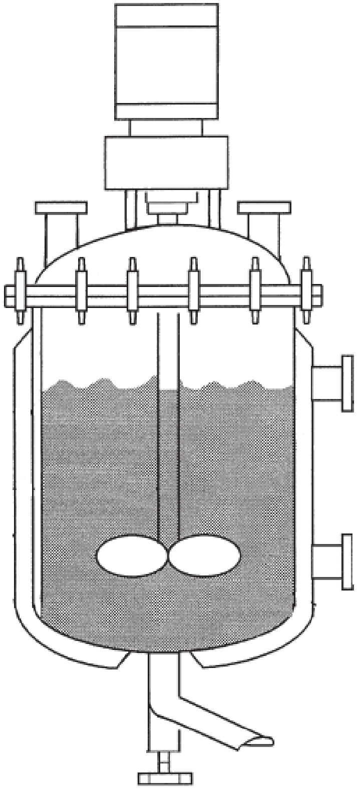
The human reactor



HCl and enzymes (E) catalyze most reactions.

The food mixes in the stomach (volume 0.5 liter), but its feed is semibatch: - a transient CSTR.

Next the acidified food passes into the small intestine (a reactor 3/4 in. in diameter and 20 ft long), where it is neutralized and mixed with more enzymes from the pancreas. This is the primary chemical reactor of the body, operating with secreted enzymes and with *E. coli bacteria catalysts.*



REACTORS occupy a central role in every chemical process

It is inside reactors a bulk of chemical transformations take place

- In typical chemical processes the capital and operating costs of the reactor may be only 10 to 25% of the total, with separation units dominating the size and cost of the process.

- Yet the performance of the chemical reactor totally controls the costs and modes of operation of these expensive separation units, and thus the chemical reactor largely controls the overall economics of most processes.

- Improvements in the reactor usually have enormous impact on upstream and downstream separation processes.

CHALLENGES ?

Chemical engineer never encounters a single reaction in an ideal single phase isothermal reactor.

Real reactors are extremely complex with multiple reactions, multiple phases, and intricate flow patterns within the reactor and in inlet and outlet streams.

An engineer needs enough information to understand the basic concepts of reactions, flow, and heat management and how these interact.

The chemical engineer almost never has kinetics for the process she or he is working on. The problem of solving the batch or continuous reactor mass-balance equations with known kinetics is much simpler than the problems encountered in practice.

Reaction rates in useful situations are seldom known, and even if these data were available, they frequently would not be particularly useful.

Many industrial processes are mass-transfer limited so that reaction kinetics are irrelevant or at least thoroughly disguised by the effects of mass and heat transfer.

Questions of catalyst poisons and promoters, activation and deactivation, and heat management dominate most industrial processes.

We usually encounter an existing reactor that may have been built decades ago, has been modified repeatedly, and operates far from the conditions of initial design. Very rarely we have the opportunity to design a reactor from scratch.

REACTION RATES?

Unfortunately, there are no tables of chemical reaction rates listed in literature.

Useful data tables and correlations can be found in areas like: thermodynamics, heat and mass transfer, or separations.

Reaction-rate data do not exist for most technologically interesting processes.

If someone claims to have a general correlation of reaction rates, the prudent engineer should be suspicious.

This is the fun (and frustration) of chemical reaction engineering.

Thermodynamics, mass and heat transfer, and separations can be said to be “finished” subjects for many engineering applications, whereas every new reaction system must be examined from first principles.

Most of the process units can be modeled and simulated using sophisticated computer programs such as ASPEN, but for the chemical reactors in a process these programs are not much help unless the kinetics are provided by the user.

The chemical reactor is the least understood and the most complex “unit” of any chemical process.

Its operation usually dominates the overall operation and controls the economics of most chemical processes.

- Systems in which chemical reactions takes place are called reactors

- **Chemical Reaction Engineering** is the engineering activity concerned with exploitation of chemical reactions on a commercial scale

Objective:

To design a reactor:

- that produces the desired product safely
- without any adverse environmental effects
- in an economical manner
- and to a desired specification

- Chemical reaction engineering involves the application of basic chemical engineering principles to the analysis and design of chemical reactors.
- Many of the operations in a chemical plant – support the chemical reactor.
- Heat exchange, separations etc. may be used to pre-treat the reactor feed and then to separate the reactor effluent into constituent parts.
- A complete understanding of reactor analysis require – knowledge & understanding of all the basic chemical engineering principles.

Scope

Design & operation of reactors

- How fast reactions occur
  Chemical Kinetics
- Maximum possible yields -TD
- Scale of operation

Calvin,Melvin

The true student will seek evidence to establish fact rather than confirm his own concept of truth, for truth exists whether it is discovered or not.

Design of reactors involve:

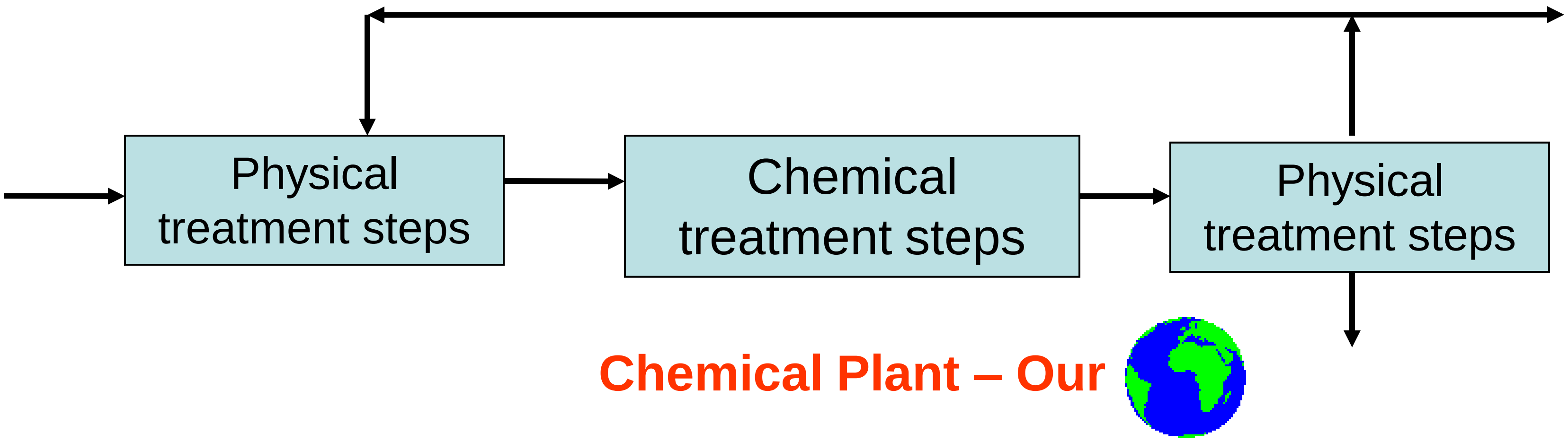
- Choosing the best type of reactor for a given reaction
- Choosing the optimum operating conditions
- Determining the Size of the reactor

The choice of reactors depends on:

- safety
- environment
- profit

Profit depends on:

- raw materials
- initial and operating costs
- market value of the finished products



- CRE deals with Chemical treatment steps

- Choice of the reactor dictates:
    - Pre and post treatment steps

Chemical reactor is the place in the process where the most value is added: lower-value feeds are converted into higher-value products.

Reactor design require

(all most all core areas of chemical engineering)

- Thermodynamics
- Chemical Kinetics
- Fluid Mechanics
- Heat & Mass transfer
- Mathematics:
- Economics

Thermodynamics

- Feasibility of a reaction
- Heat of reaction, effect of temperature
- Equilibrium yields, constant, composition

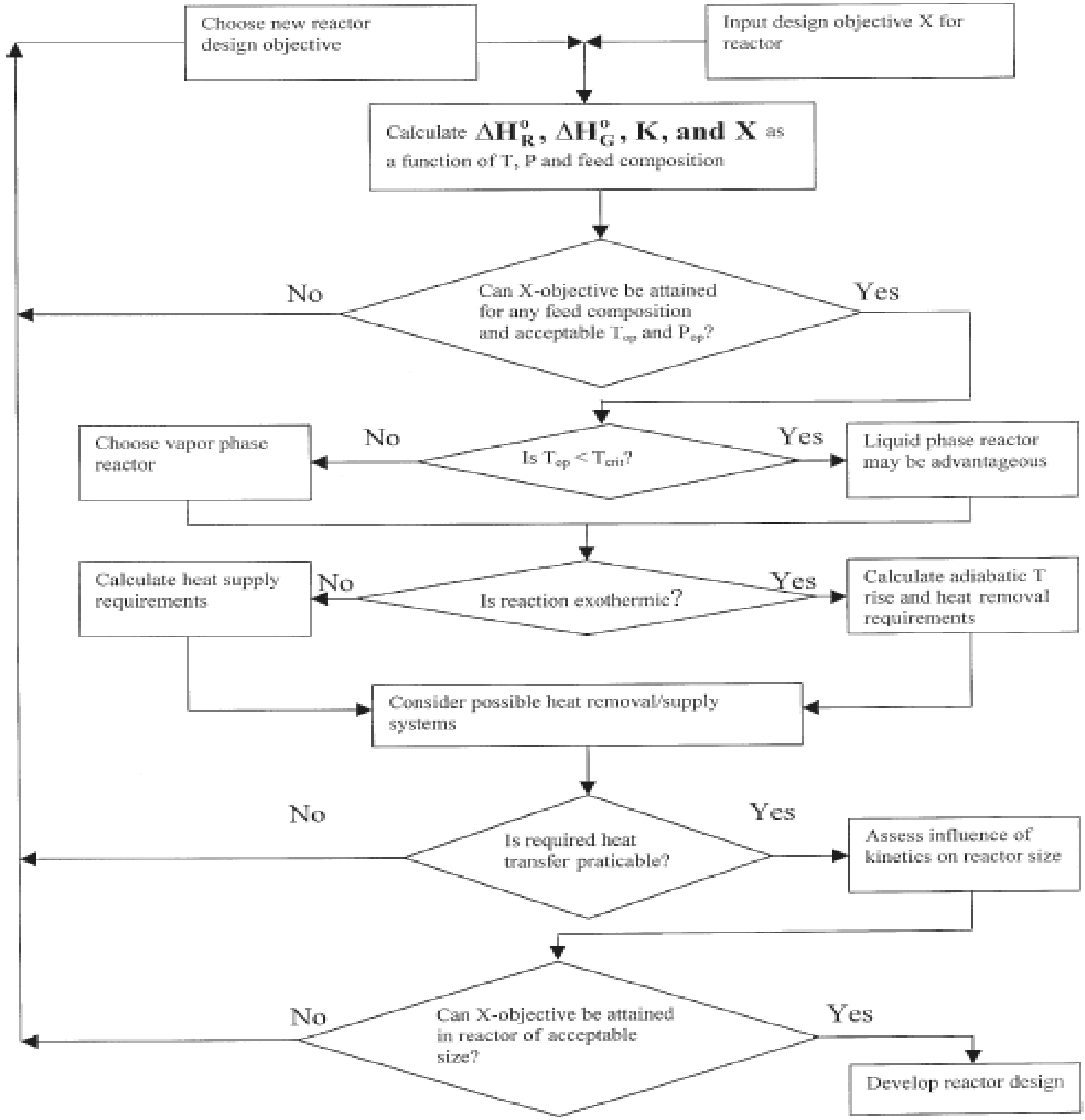
Chemical Kinetics

- Quantitative studies of the rates at which chemical processes occur
- Factors on which these rates depend
- Reaction mechanism

A description of a reaction in terms of its constituent molecular acts is known as the mechanism of the reaction.

Chemical Kinetics & Thermodynamics

- Time is a variable in kinetics but not in thermodynamics; TD does not deal with respect to time; equilibrium is a time-independent state.
- Information about the mechanism of chemical change can be obtained from kinetics but not from thermodynamics.
- The rate of chemical change is dependent on the path of reaction; thermodynamics is concerned with "state" and change of state of a system.
- Chemical kinetics is concerned with the rate of reaction and factors affecting the rate, and chemical thermodynamics is concerned with the position of equilibrium and factors affecting equilibrium.



Flowchart for reactor design

Liquid phase over the gas phase operation

Advantages:

- For the desired product the reactor may be smaller
- The heat capacities and thermal conductivities are greater for liquids - factors which increase the heat transfer
- The equipment size is small resulting in lower power requirements and capital costs.

Disadvantages:

- corrosion and catalyst losses.
- In considering a liquid system, all operating conditions must fall within the two-phase region
- high operating pressures are potentially hazardous and expensive to contain

How to say a chemical reaction has occurred ?

A chemical species is said to have reacted when it has lost its chemical identity. The identity of a chemical species is determined by the *kind, number,* and *configuration* of that species' atoms.

Three ways a chemical species can lose its chemical identity:

1. Decomposition $C_2H_5CH = CH_2 \rightarrow CH_2 = C(CH_3)_2$

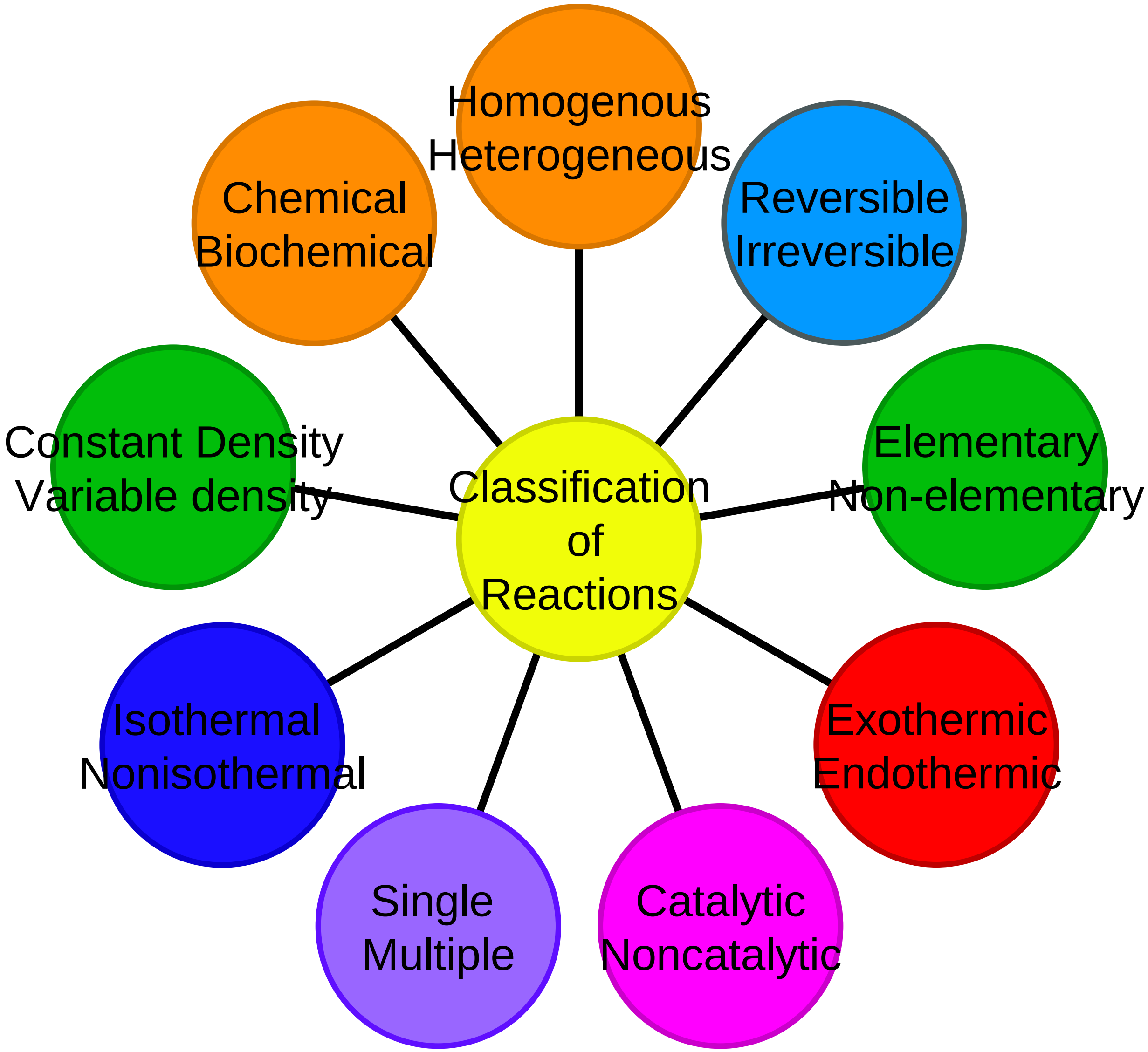
2. Combination $N_2 + O_2 \rightarrow 2NO$

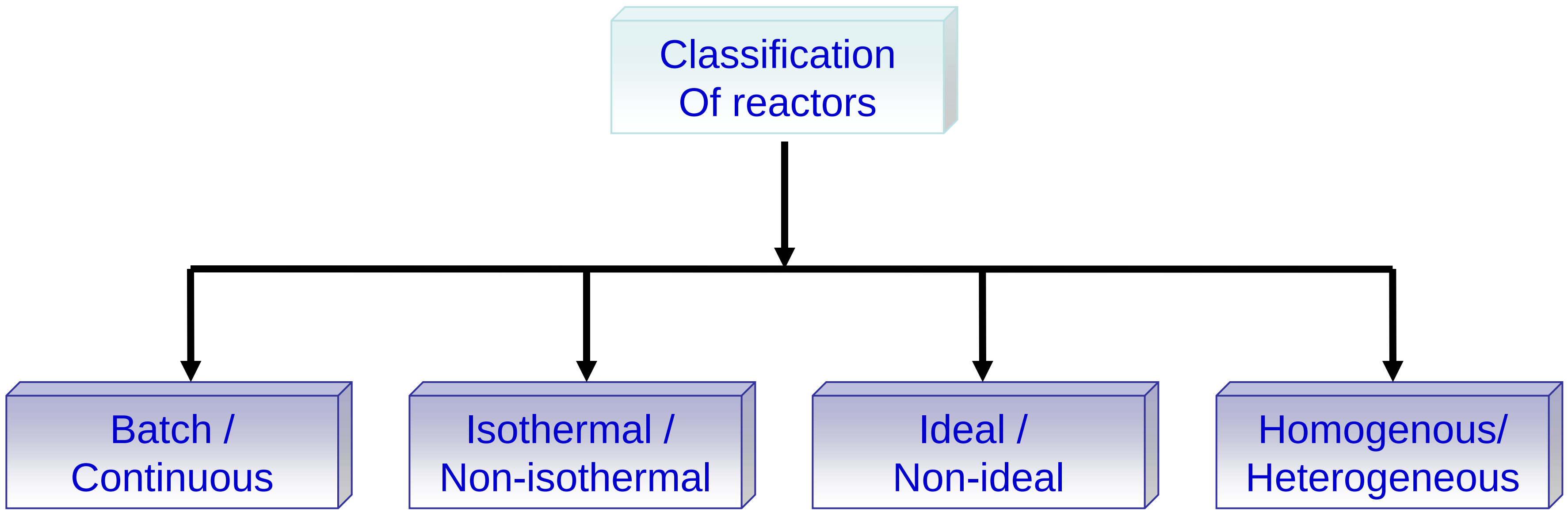
3. Isomerization $CH_3CH_3 \rightarrow H_2 + H_2C = CH_2$

Quiz

During a Chemical Reaction

- Is mass conserved ?
- Are moles conserved ?
- Is energy conserved ?
- Is volume/density conserved ?


Homogenous
Heterogeneous
Chemical
Biochemical
Reversible
Irreversible
Constant Density
Variable density
Classification
of
Reactions
Elementary
Non-elementary
Isothermal
Nonisothermal
Exothermic
Endothermic
Single
Multiple
Catalytic
Noncatalytic


Classification
Of reactors
Batch /
Continuous
Isothermal /
Non-isothermal
Ideal /
Non-ideal
Homogenous/
Heterogeneous

Non–Ideal

Non-isothermal

Heterogeneous React

Multiple Reactors

Multiple Reactions

Variable density

Constant density

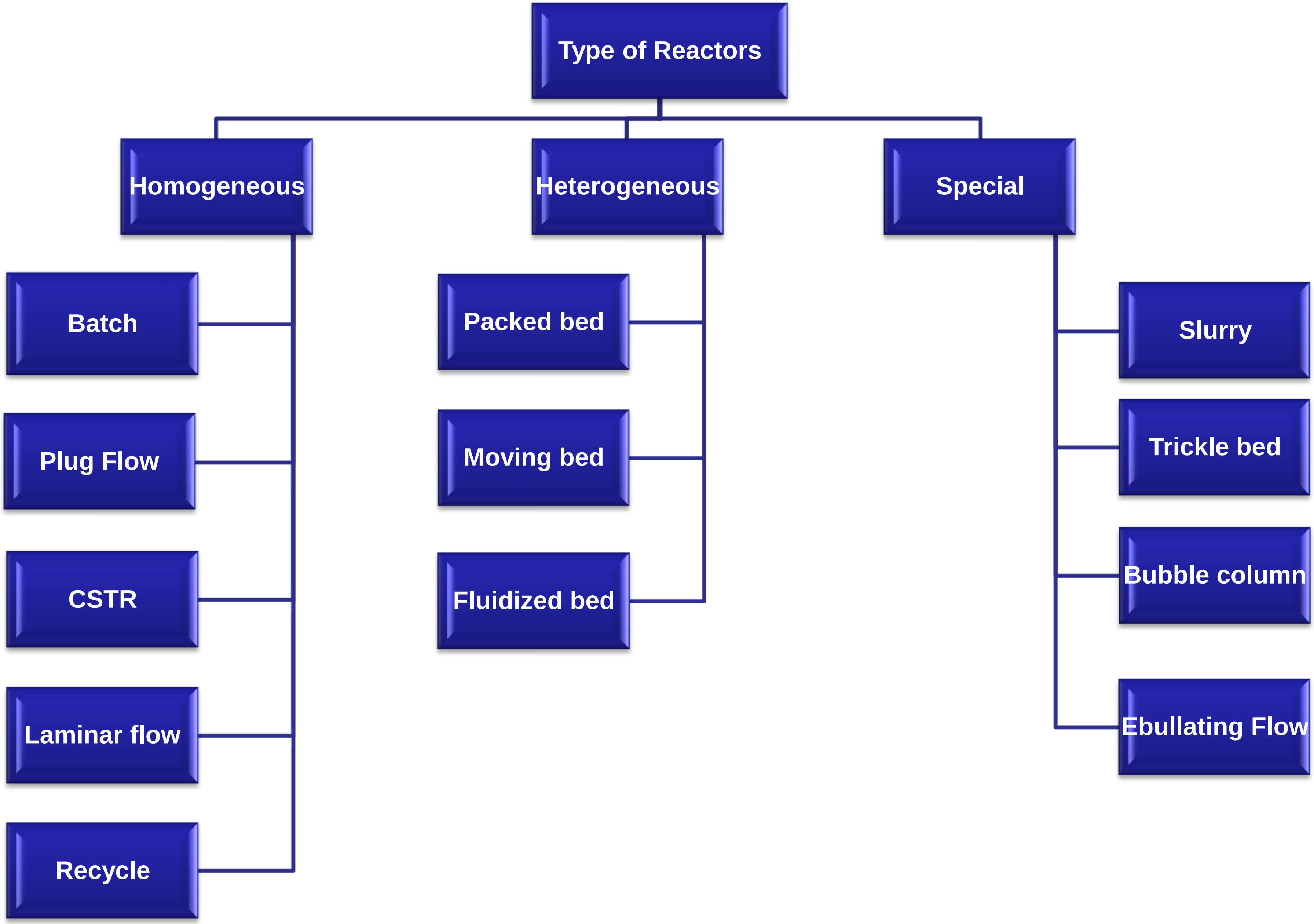
Isothermal Reactors

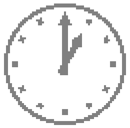
Homogen. Reactors

Single Reactions

Ideal Reactors

Uphill Task


Type of Reactors
Homogeneous
Heterogeneous
Special
Batch
Plug Flow
CSTR
Laminar flow
Recycle
Packed bed
Moving bed
Fluidized bed
Slurry
Trickle bed
Bubble column
Ebullating Flow



Time line ….

- 1777 *Wenzel* - first quantitative data on rates of reactions
- 1796 *Van Narum* – first to recognize catalysis
- 1867 *Guldberg & Waage* – law of mass action for homogeneous reactions
- 1877 *Van't Hoff* – extended to heterogeneous reactions
- 1889 *Arrhenius* – concept of activation energy
- 1902 *Ostwald* – definition of catalyst
- 1920 *Taylor* – active site catalytic action
- 1923 *Lewis & Ries* – use of reaction kinetics in the design of reactors
- 1950 Dankwerts – structure of RTD for analysis

Any Questions?

"There is an important question that must be asked when approaching any difficult project for the first time, and that question is, "Why bother?"