# Chemical Reaction Engineering

Jayant M. Modak
Department of Chemical Engineering
Indian Institute of Science, Bangalore

# About Chemical Reaction Engineering and Engineer

- **One feature that distinguishes the education of Chemical Engineer from that of other Engineer is an exposure to the basic concepts of Chemical Reaction Engineering**

**Charles Hill, *An Introduction to Chemical Engineering Kinetics and Reactor Design***

# About Chemical Reaction Engineering and Engineer

- Chemical Reaction Engineering is that engineering activity which is concerned with the exploitations of Chemical Reactions on a Commercial Scale

**Octave Levenspiel, *Chemical Reaction Engineering***

# About Chemical Reaction Engineering and Engineer

- **Typical tasks of Chemical Engineer are**
  - **Design of Chemical Processes**
  - **Maintain and Operate a process**
  - **Fix some perceived problems**
  - **Increase capacity or selectivity at minimum cost**

**Lanny Schmidt, *The Engineering of Chemical Reactions***

# Scope of Chemical Reaction Engineering

- petroleum refining, petrochemicals, chemicals, and pharmaceuticals
- biotechnology, microelectronics, advanced materials, and energy from non-fossil resources
- environment, pollution prevention, sustainable development

# Chemical Reaction Engineering – New frontiers

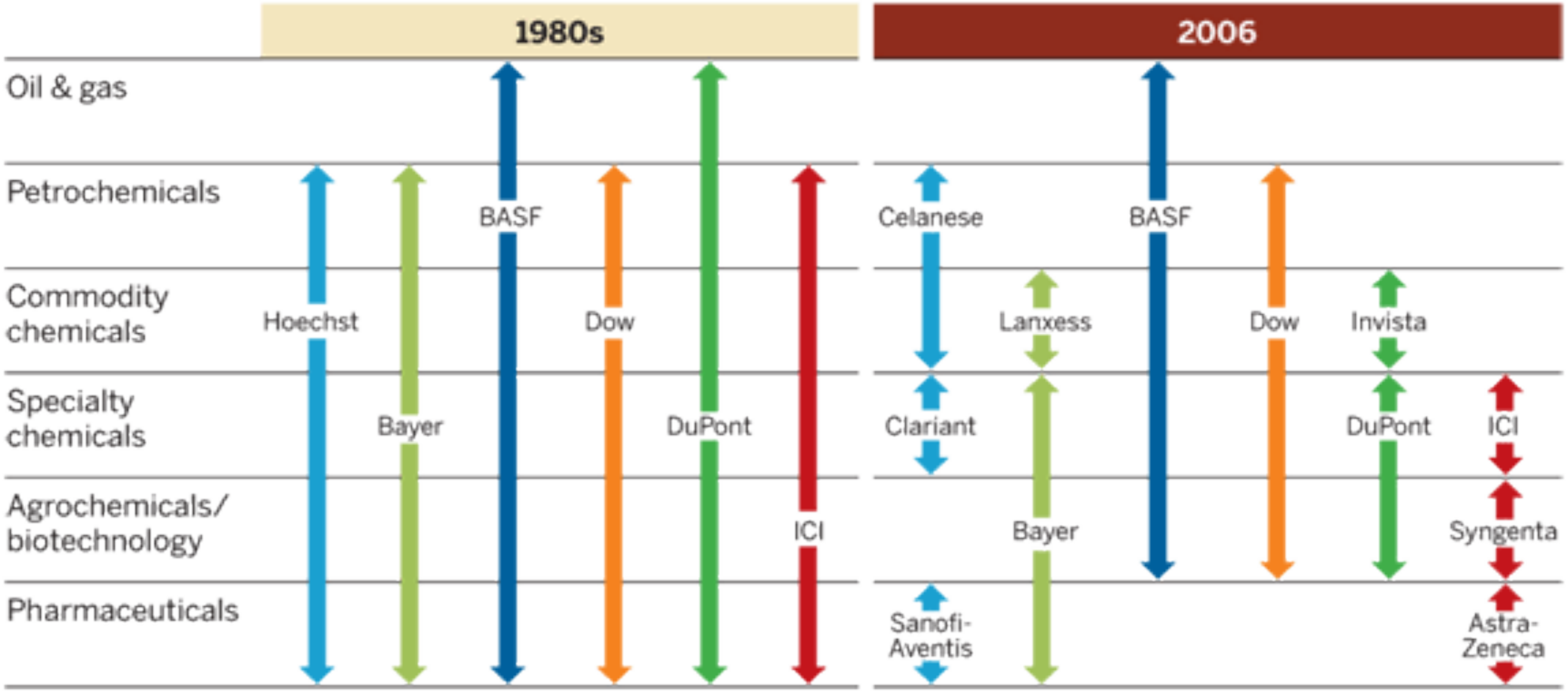
- New analytical instrumentation providing quantitative information on species and mechanisms
- New computational resources – hardware and software
- Multiscale approach

# Top Global Players in 2008

| Rank | Company | Sales $ bn |
|---|---|---|
| 1 | BASF (Germany) | 70.5 |
| 2 | DOW (U.S.) | 57.5 |
| 3 | Ineos (UK) | 36 |
| 4 | LyondalBasell | 38.4 |
| 5 | ExxonMobile Chemicals (USA) | 38.4 |
| 27 | Reliance Industries (India) | 12.6 |

*Chemical & Engineering News, August 2009*

# Narrowing In




**SOURCE:** BASF

*Chemical & Engineering News, July 2007*

## *Chemical Industry Sectors*

| Category | Typical Plant (TPA) | Price ($/kg) | E-Factor (Kg/Kg) |
|---|---|---|---|
| Petroleum Refining | $10^6$ - $10^8$ | 0.05 | 0.1 |
| Commodity chemicals | $10^4$ - $10^6$ | 0.05-1 | 1-3 |
| Fine chemicals | $10^2$ - $10^4$ | 1-5 | 2-10 |
| Foods | | 0.5-25 | |
| Materials | | 0- .... | |
| Pharmaceuticals | 10 - $10^3$ | 10 - ...... | 10-100 |
| Electronic chemicals, Environment, Neutraceuticals, Chiral and Biopharmaceuticals, | | | |

**Lanny Schmidt,** *The Engineering of Chemical Reactions*

## *What do you we need to know about chemical processes?*

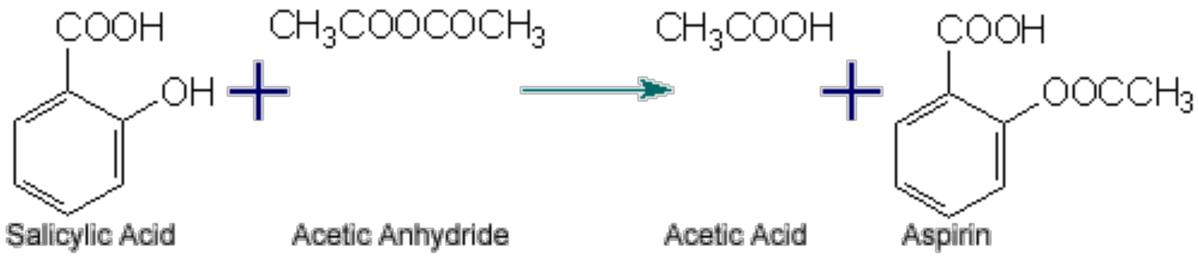
**Chemistry is important**

**A + B - > C + D is not a real reaction**

**Example: Ammonia synthesis**

$$N -- N + 3\ H -- H \leftrightarrow 2\ N -- H_3$$

**Example: aspirin synthesis**




**Lanny Schmidt,** *The Engineering of Chemical Reactions*

## *What do you we need to know about chemical processes?*

**Single reaction in an ideal single phase isothermal reactor is hardly encountered. Real reactors are extremely complex with multiple reactions multiple phases and intricate flow patterns**

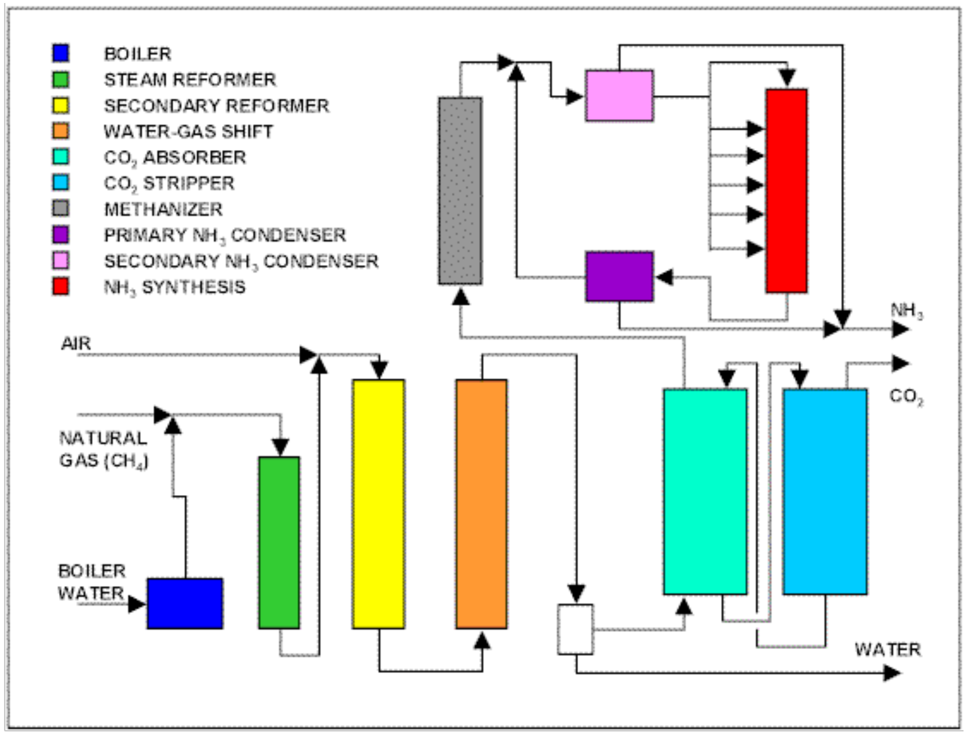
**Example: Ethylene synthesis**

$$C_2H_6 \rightarrow C_2H_4 + H_2$$
$$C_2H_6 \rightarrow C_2H_2 + H_2$$
$$3\ C_2H_6 \rightarrow C_6H_6 + 6\ H_2$$
$$C_2H_6 \rightarrow 2\ C + 3\ H_2$$

## *What do you we need to know about chemical processes?*

### Example: Ammonia synthesis

$$CH_4 + H_2O \rightarrow CO + 3\ H_2$$
$$N_2 + 3\ H_2 \leftrightarrow 2\ NH_3$$



## *What do you we need to know about chemical processes?*

**Reactions with simple kinetics are extremely rare.**

**Example: Ammonia synthesis**

$$r_{2+} - r_{2-} = K_1 k_2 \left[ \left( \frac{p_{N_2}}{p^{\circ}} \right) - \frac{\left( \frac{p_{NH_3}}{p^{\circ}} \right)^2}{K_g \left( \frac{p_{H_2}}{p^{\circ}} \right)^3} \right] \theta_*^2$$

$$\theta_* = \frac{1}{1 + K_1 \frac{p_{N_2}}{p^{\circ}} + \frac{\frac{p_{NH_3}}{p^{\circ}}}{K_3 K_4 K_5 K_6 \; K_7^{3/2} \left( \frac{p_{H_2}}{p^{\circ}} \right)^{3/2}} + \frac{\frac{p_{NH_3}}{p^{\circ}}}{K_4 K_5 K_6 K_7 \frac{p_{H_2}}{p^{\circ}}} + \frac{\frac{p_{NH_3}}{p^{\circ}}}{K_5 K_6 \; K_7^{1/2} \left( \frac{p_{H_2}}{p^{\circ}} \right)^{1/2}} + \frac{\frac{p_{NH_3}}{p^{\circ}}}{K_6} + K_7^{1/2} \left( \frac{p_{H_2}}{p^{\circ}} \right)^{1/2}}$$

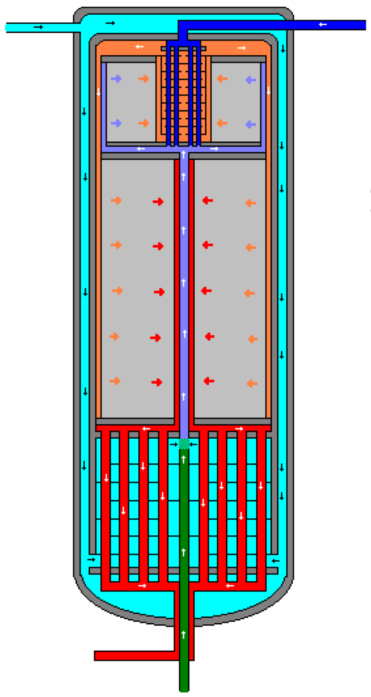
# *Most industrial processes are heterogeneous*

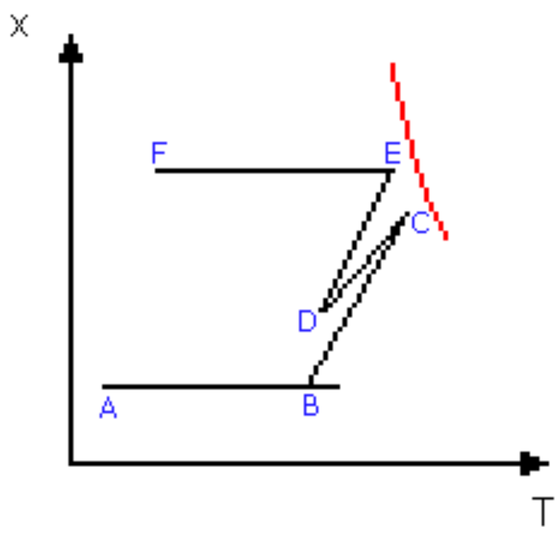
| Process | Reaction | Conditions | Reactor | Comments |
|---|---|---|---|---|
| Catalytic naptha reforming | Naptha (?) → aromatics<br>Endothermic | 350-4000 kPa<br>490-525 C<br>$Pt\text{-}Al_2O_3$<br>G-S, | Fixed Bed | Catalyst deactivation<br>Regeneration |
| $NO_x$ Absorption | $2\ NO + O_2 \rightarrow 2\ NO_2$ (G)<br>$NO_2$ (G) → $NO_2$ (L)<br>$2\ NO_2 + H_2O \rightarrow HNO_2 + HNO_3$ (L) | 1 Atm<br>25-30 C<br>G-L | Packed tower | |
| Chemical Vapor Deposition | $SiCl_4 + H_2 \rightarrow Si$ (S) + 4 HCl | $10^{-6}$ - $10^{-3}$ atm<br>1000-1200 C<br>micron thickness<br>G-S | Chamber reactors | Uniformity essential<br>Flow past plate |
| Antibiotics Production | Glucose → Penicillin<br>Exothermic | 1 atm, 30 C<br>microbial cells<br>G-L-C | Stirred tank reactors | Living |

# *Transport processes are important*

| | |
|---|---|
| Ammonia Reactor - 1500 t NH3/day, 100 $m^3$ volume, 250 t of catalyst. | Catalyst - Fe with K and $Al_2O_3$ |

# *Industrial reactors have intricate flow patterns*






**A** : The main flow (pale blue) first flows along the pressure shell and cools it.

**B :** In the first bed, both the temperature and the concentration increases.

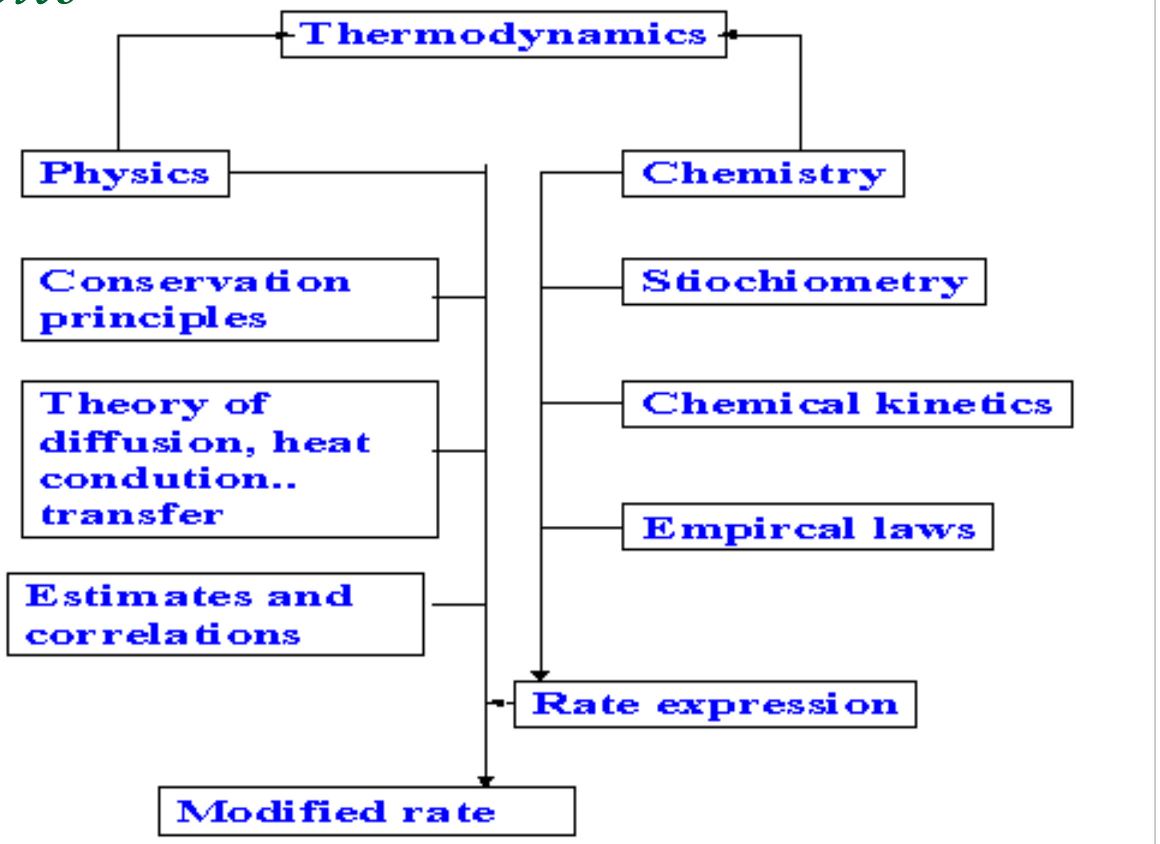
**C :** The gas is cooled in the upper heat exchanger and the third inlet gas stream (dark blue) is added.

**D :** In the second bed, both the temperature and the concentration increases.

# *Summary - Chemical Reactor Analysis*

*R. Aris, Ind. & Eng. Chemistry, 56, p.22, 1964*

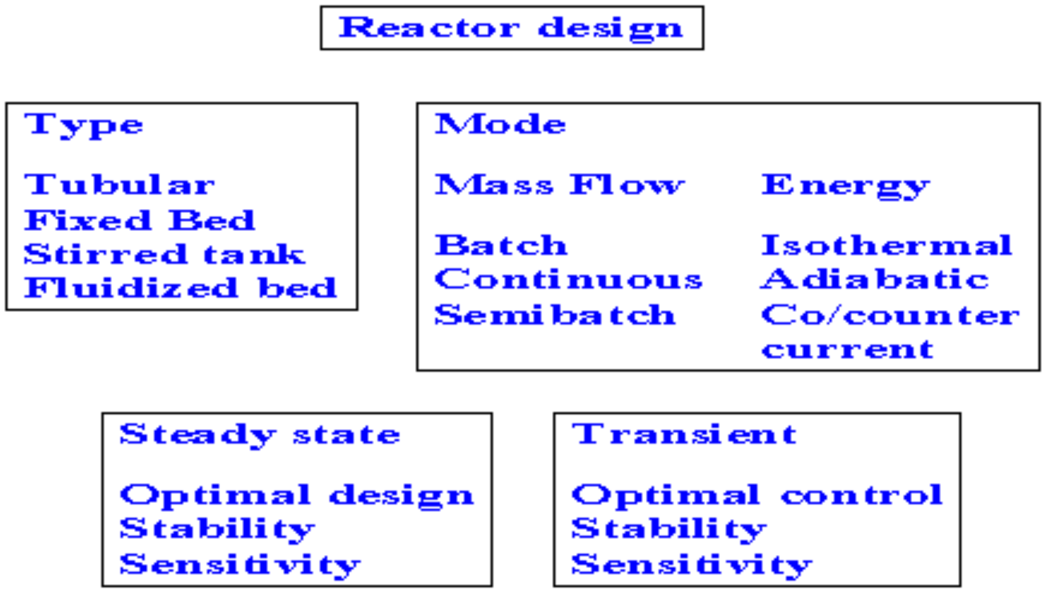
## *Step 1 - Kinetics*



# *Summary - Chemical Reactor Analysis*

*R. Aris, Ind. & Eng. Chemistry, 56, p.22, 1964*

## *Step 2 – Reactor design*



# Course outline

| Topic |
|---|
| 1. Review of undergraduate reaction engineering:<br><br>Stoichiometry, thermodynamics of reacting systems, kinetics of elementary reactions, ideal reactors: CSTR/ PFR |
| 2. Kinetics of complex reactions:<br><br>Reaction mechanism and kinetics, Chain, catalytic, polymerization, biochemical reactions, Analysis of reaction network, lumping analysis, Parameter estimation |

# Course outline

| Topic |
| --- |
| 3. Conservation equations for chemically reacting mixtures |
| 4. Heterogeneous reactions:<br><br>Mass transport with reaction, Catalytic and Non-catalytic gas-solid reactions, Gas-liquid reactions |
| 5. Chemical Reactor Design:<br><br>Transient and steady state analysis, Optimal design of reactors, Multiphase reactors: fixed, fluidized, trickle bed, slurry etc, Non-ideal continuous flow reactors |

# Course Textbooks/Reference

- Aris R., Elementary Chemical Reactor Analysis, Prentice-Hall 1969.
- Foggler, H. S., Elements of Chemical Reaction Engineering, Prentice Hall of India, 1994.
- Froment G.F. and Bischoff K.B., Chemical Reactor Analysis and Design, John Wiley 1994.
- Schimdt L., The Engineering of Chemical Reactions, Oxford, 2005