Chemical Reaction Engineering
Reactor Design

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Chemical Reactor Design

➢ **Objectives**

- ❑ **Technological**
  - ■ Maximum possible product in minimum time
  - ■ Desired quantity in minimum time
  - ■ Maximum possible product in desired time

- ❑ **Economic**
  - ■ Maximize profit

Chemical Reactor Design

- ➤ **Constraints**
  - ❑ Market
    - ■ Raw materials availability – quality and quantity
    - ■ Demand for the product
  - ❑ Society/Legislative
    - ■ Safety
    - ■ Pollution control
  - ❑ Technological
    - ■ Thermodynamics
    - ■ Stoichiometry
    - ■ Kinetics

Chemical Reactor Design - Decisions

- ➤ Type of reactor
  - ❑ Tubular, Fixed Bed, Stirred tank, Fluidized bed
- ➤ Mode
  - ❑ Mass Flow: Batch, Continuous, Semibatch
  - ❑ Energy: Isothermal, Adiabatic, Co/counter current
- ➤ Process Intensification
  - ❑ Combining more than one type of unit operation

Tubular reactor – mass balance

$$\frac{\partial C_j}{\partial t} + \frac{\partial}{\partial z}\left(Flux_j\right) = R_j \qquad\qquad \frac{\partial C_j}{\partial t} + \frac{\partial}{\partial z}\left(uC_j + J_j\right) = R_j$$

$$\frac{\partial}{\partial t}\left(\sum_j M_j C_j\right) + \frac{\partial}{\partial z}\left(u\sum_j M_j C_j + \sum_j M_j J_j\right) = \sum_j M_j R_j$$

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial}{\partial x}\left(u\rho_f\right) = 0$$

Tubular reactor – energy balance

$$\frac{\partial}{\partial t}(C_T U) + \frac{1}{A}\frac{\partial}{\partial z}\left(F_T H + A\sum_j H_j J_j\right) = Q$$

$$\frac{\partial}{\partial t}(C_T U) = \frac{\partial}{\partial t}(C_T H - P) = \left(\sum_j H_j\right)\frac{\partial C_j}{\partial t} + \left(\sum_j C_j C_{P_j}\right)\frac{\partial T}{\partial t}$$

$$\frac{\partial}{\partial z}(F_T H) = \left(\sum_j H_j\right)\frac{\partial F_j}{\partial z} + \left(\sum_j F_j C_{P_j}\right)\frac{\partial T}{\partial z}$$

$$\frac{\partial}{\partial z}\left(\sum_j H_j J_j\right) = \left(\sum_j H_j\right)\frac{\partial J_j}{\partial z} + \left(\sum_j J_j\right)\frac{\partial H_j}{\partial z}$$

Tubular reactor – energy balance

$$\left(\sum_j H_j\right)\left(\frac{\partial C_j}{\partial t} + \frac{1}{A}\left[\frac{\partial F_j}{\partial z} + A\frac{\partial J_j}{\partial z}\right]\right) = \left(\sum_j H_j R_j\right) = \sum_i \Delta H_i\, r_i$$

$$\left(\sum_j C_j C_{P_j}\right)\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial u}\right)$$

$$Q = \frac{4}{d_t}U\left(T_r - T\right)$$

$$\left(\sum_j C_j C_{P_j}\right)\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial u}\right) + \sum_i \Delta H_i\, r_i = \frac{4}{d_t}U\left(T_r - T\right)$$

Stirred tank reactor – mass and energy balance

$$\frac{dN_j}{dt} = F_{j0} - F_{je} + R_j$$

$$\left(\sum_j N_j C_{P_j}\right)\frac{dT}{dt} = \sum_j F_{j0}\left(H_{j0} - H_{je}\right) + V\sum_i(-\Delta H_i)r_i + A_K U\left(T_r - T\right)$$

Fixed bed reactor – mass balance

$$\frac{\partial}{\partial t}\left(\varepsilon_B C_j\right) + \frac{\partial}{\partial z}\left(\varepsilon_B Flux_j\right) = q_{mj}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_B C_j\right) + \frac{\partial}{\partial z}\left(u_s C_j - D_{ej,s}\rho_f \frac{\partial}{\partial z}\left(\frac{C_j}{\rho_f}\right)\right) = q_{mj}$$

$$\left(\sum_j C_j C_{P_j}\right)\left(\frac{\partial T}{\partial t} + u_s \frac{\partial T}{\partial z} - \lambda_e \frac{\partial^2 T}{\partial z^2}\right) + q_h = \frac{4}{d_t}U\left(T_r - T\right)$$

$$\frac{1}{r}\frac{\partial}{\partial}\left(rX\frac{\partial Y}{\partial r}\right) \quad (X,Y) = \left|\begin{matrix}\left(D_{ej,r}, C_j\right)\\ \left(\lambda_{e,r}, T\right)\end{matrix}\right.$$

Psuedohomogenous model

$$q_{mj} = R_j$$

$$q_h = \sum_i \Delta H_i \, r_i$$

Heterogenous model – external diffusion

$$q_{mj} = -K_g(C_j - C_{js}) \cdot g \cdot g A_p = -K_g a_v(C_j - C_{js})$$

$$a_v = \frac{3}{R}(1 - \varepsilon_B)$$

$$q_h = h_f a_v (T - T_s)$$

$$K_g a_v(C_j - C_{js}) = -R_j\left(C_{js}, T_s\right)$$

$$h_f a_v (T - T_s) = \sum_i \Delta H_i \, r_i$$

Heterogenous model – internal diffusion

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_{ej}^{'}\frac{\partial C_{j}^{'}}{\partial r}\right) = -R_{j}^{'}\left(C_{j}^{'}, T^{'}\right)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \lambda_{e}^{'}\frac{\partial T^{'}}{\partial r}\right) = \sum_{i}\Delta H_{i}\, r_{i}^{'}$$

$$q_{mj} = -D_{ej}^{'}\left.\frac{\partial C_{j}^{'}}{\partial r}\right|_{r=R} \qquad a_{v} = \eta R_{j}\left(C_{j}\right)$$

$$q_{h} = \sum_{i}\eta_{i}\left(-\Delta H_{i}\right)r_{i}$$

Non-isothermal reactors - PFR

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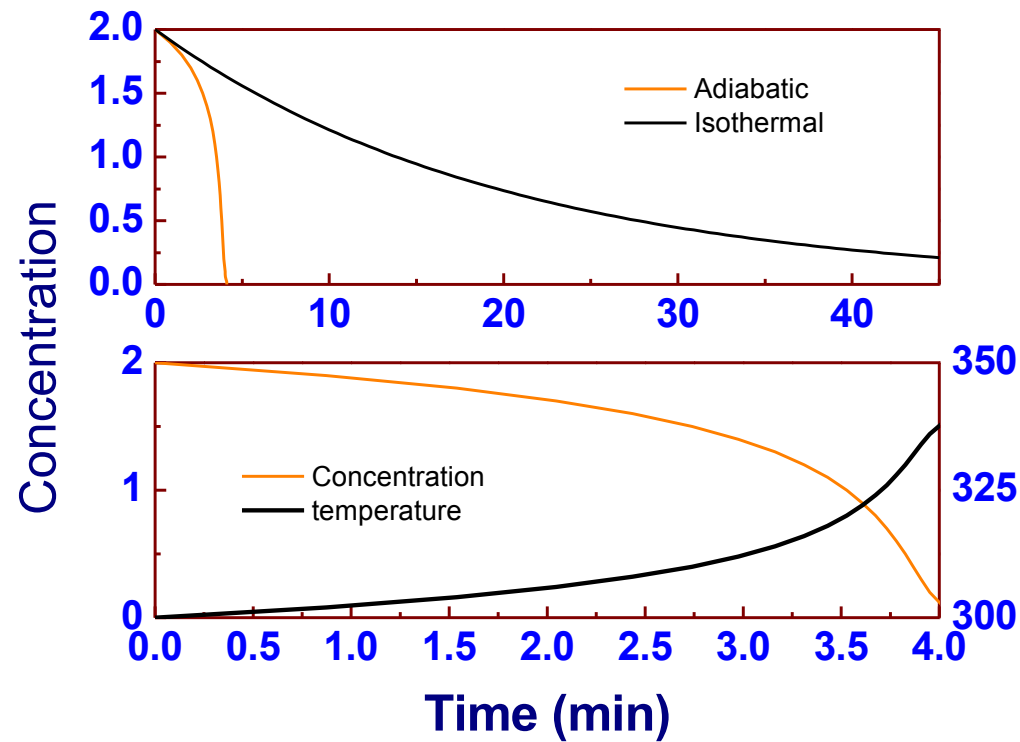
Non-isothermal reactors - CSTR

Non-isothermal reactors - rate
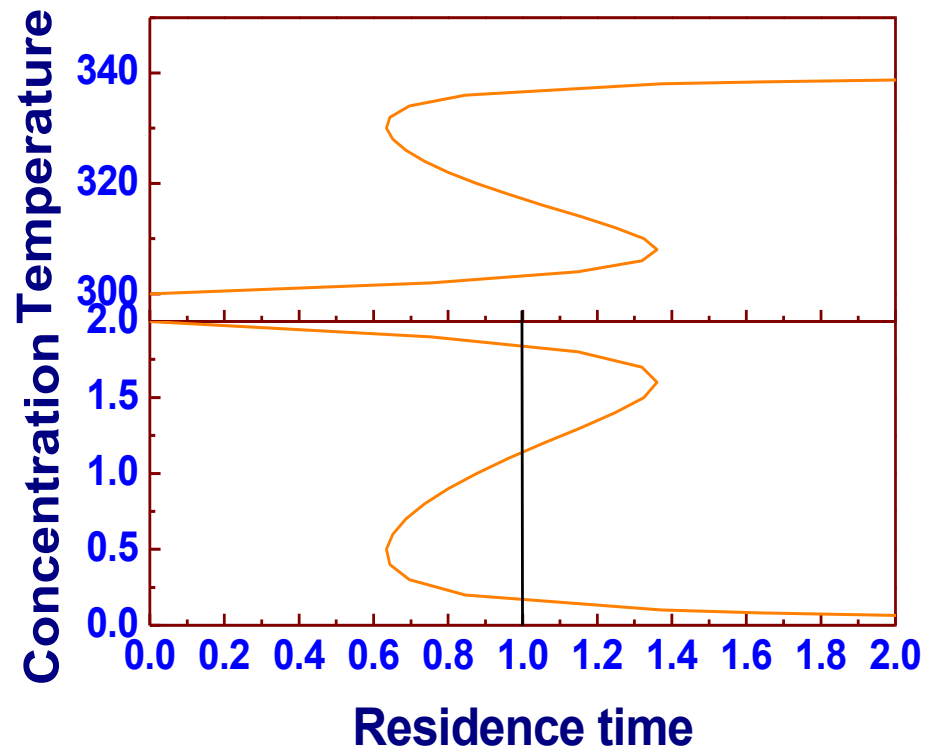
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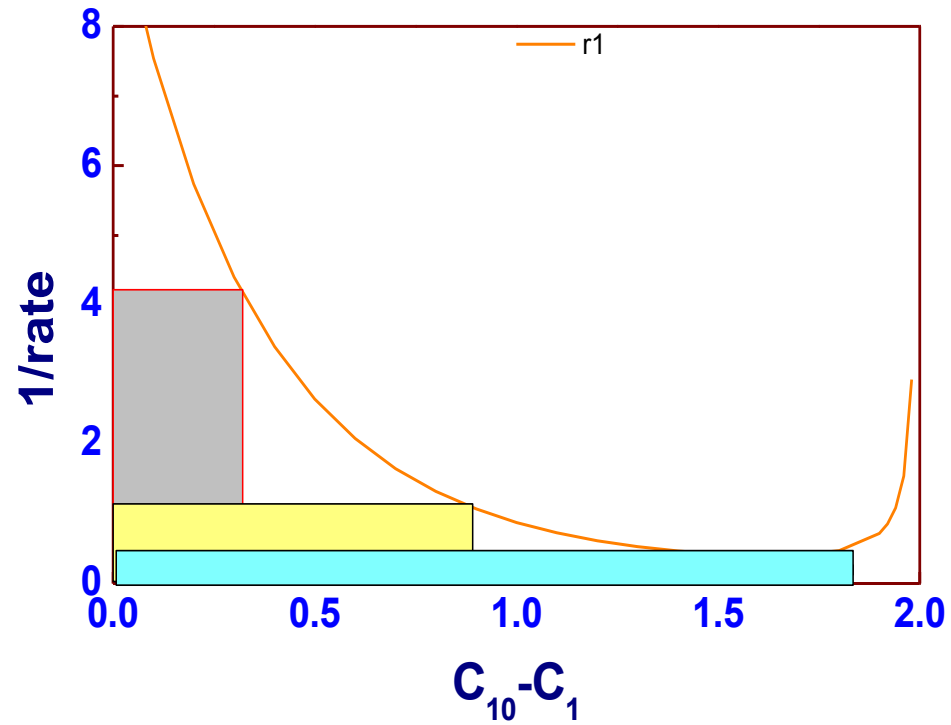
Trajectories - Exothermic reaction
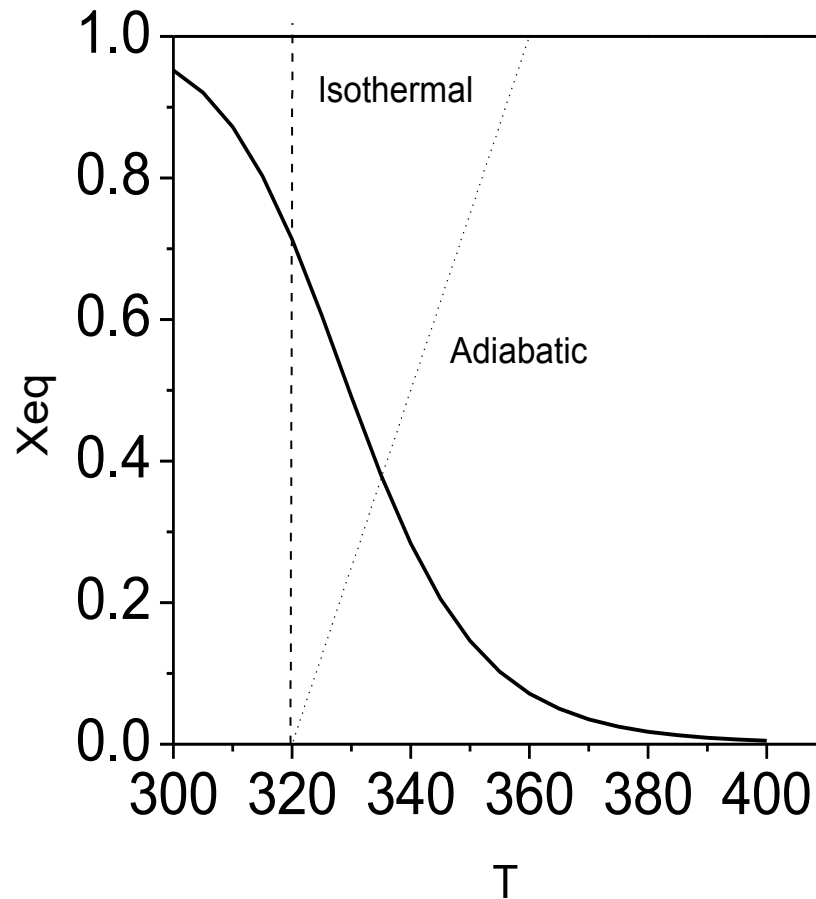
Trajectories - Endothermic reaction
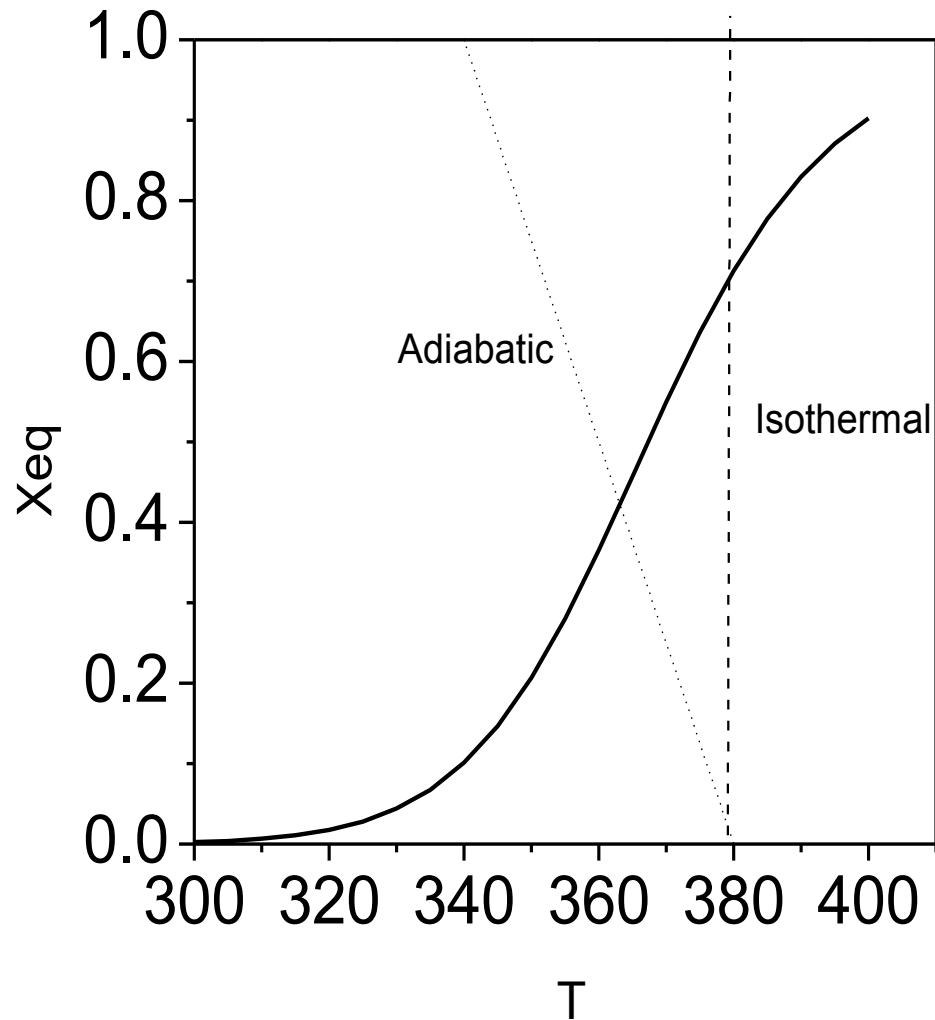
Optimal temperature trajectories
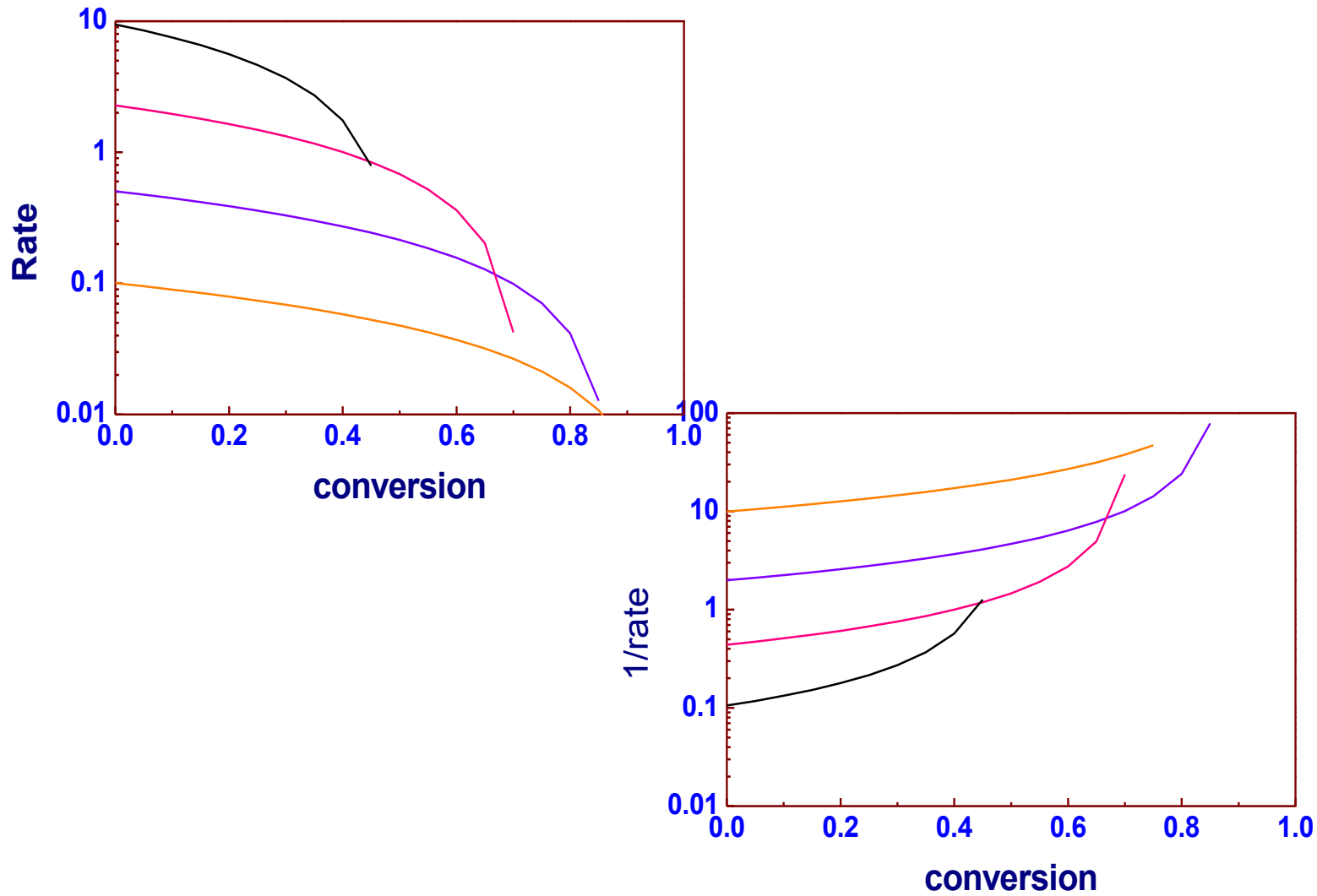
Optimal temperature
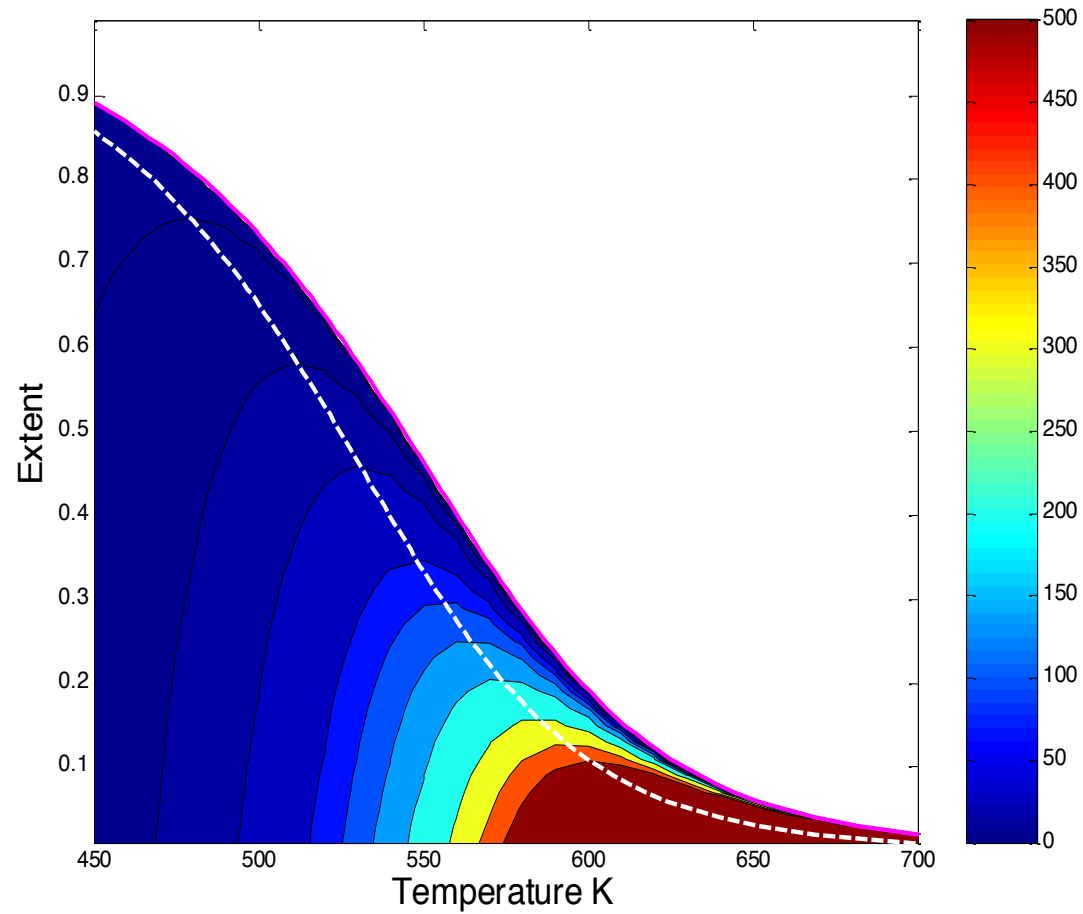
Thermal cracking of ethane in tubular reactor

- Ethylene demands – polyethylene, ethylene oxide, ethylene glycol – 20 million tons per annum

- Main Reaction $C_2H_6 \rightarrow C_2H_4 + H_2$ increase in number of moles so steam as inert

- Endothermic reaction - ΔH 34.5 kcal/mol, high temperature for high equilibrium conversions, increasing temperatures along the length of the reactor

$$2C_2H_6 \rightarrow C_3H_8 + CH_4$$

- Side reactions higher conversion yield of side products higher

Yield conversion diagram for ethane cracking
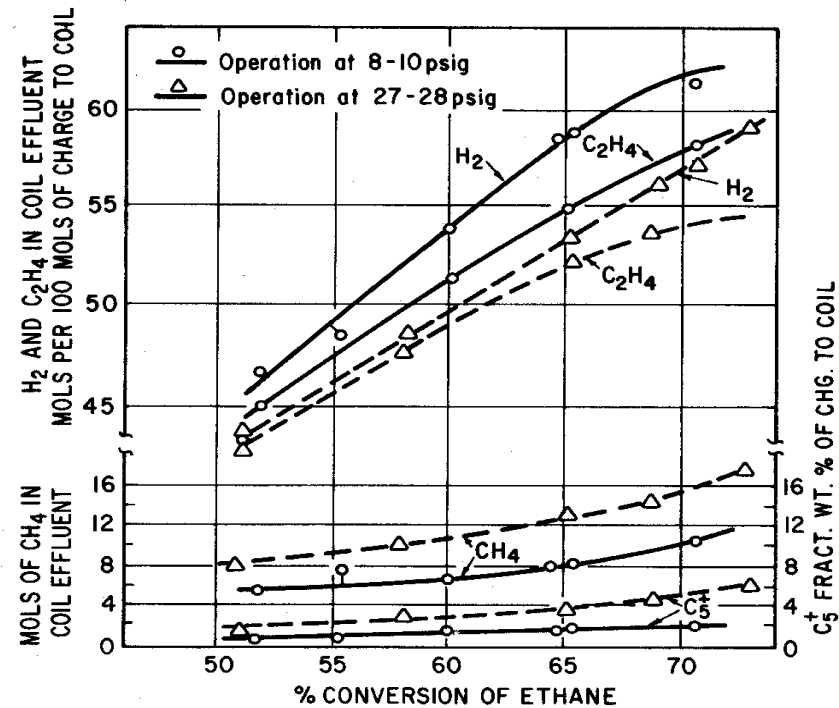
Fig. 10.15 Product distribution for ethane pyrolysis (1490–1530°F). Adapted by permission: H. C. Schutt, *Chem. Eng. Prog.,* **55** (1), 68 (1959).

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Ethane cracking reactor
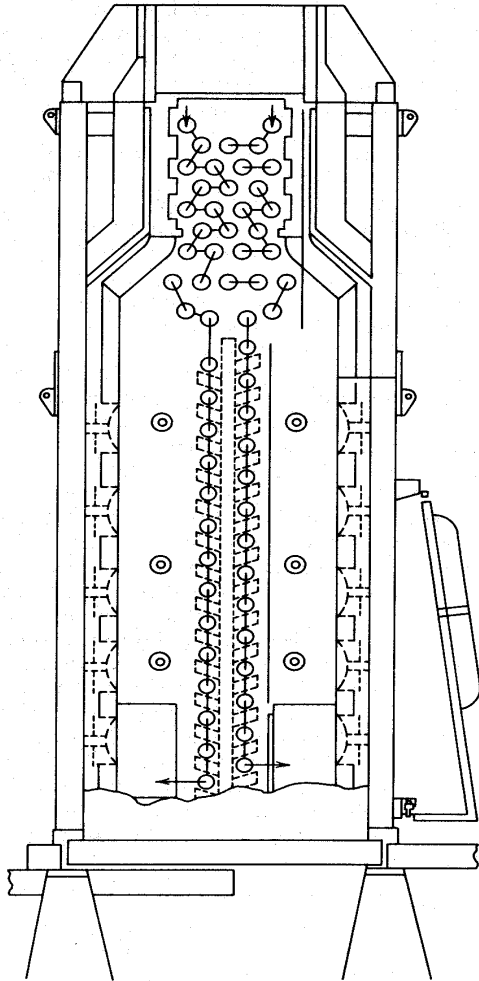
Figure 1 Configuration of ethane furnace.

Typical operating condn

• L = 95 m

• G = 68.68 kg/m2/s

• P inlet 2.99 atm, outlet 1.2 atm

• T inlet 680, outlet 820 C

• Production 10000 tons/coil

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Balances

$$\text{mass} \quad \frac{dF_j}{dz} = R_j \frac{\pi d_t^2}{4}$$

$$\text{energy} \quad \frac{dT}{dz} = \frac{1}{\sum_j F_j C_{pj}} \left[q(z) \pi d_t + \frac{\pi d_t^2}{4} \sum_i -(\Delta H_i) r_i \right]$$

$$\text{momentum} \quad -\frac{dp}{dz} = \left[\frac{2f}{d_t} + \frac{\xi}{\pi r_{b\,i}} \right] \rho_f u^2 + \rho_f u \frac{du}{dz}$$

$$u = \frac{F'}{A} = \frac{1}{A} \left[\frac{RT \sum_j F_j}{p} \right]$$

Simulation of ethane reactor
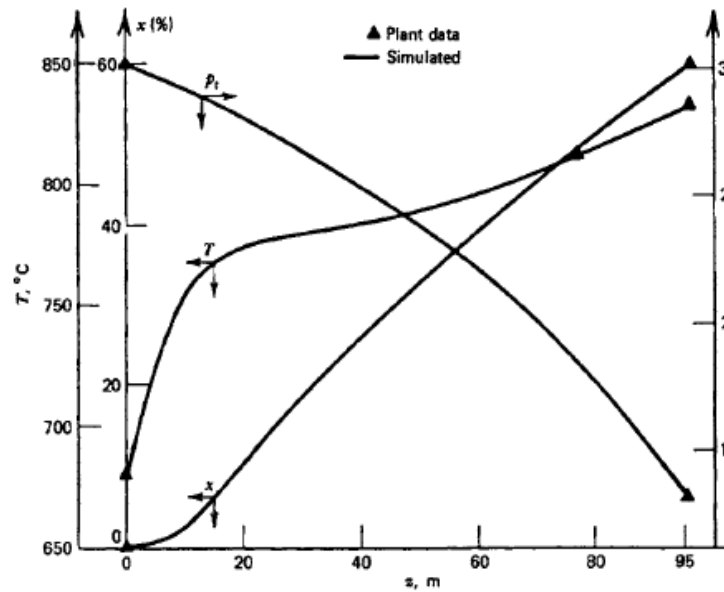
Figure 2 Ethane cracking. Reactor simulation.
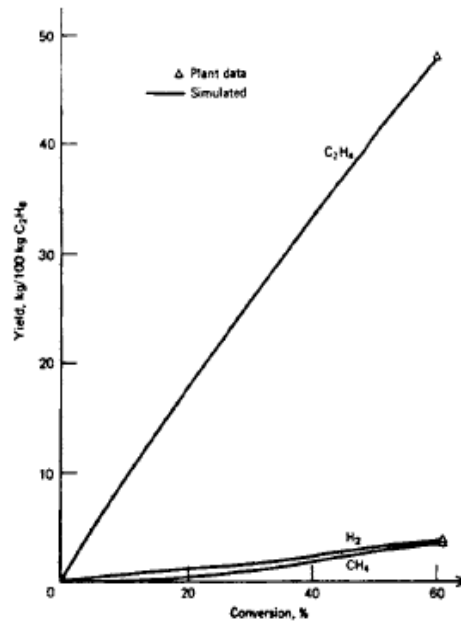
Figure 3 Ethane cracking. Product distribution.

Hydrogenation of oil

- ➢ Major demand – margarine, shortenings, vanaspati

- ➢ Vegetable oils – mixture of triglycerides - glycerol and fatty acids

- ➢ Fatty acids – saturated (S) , monosaturated (cis, R1 and trans, R2) and diunsaturated (B). Hydrogenation to reduce odor or color, improve stability and increase melting point.

- ➢ Product requirements – some polyunsaturated (health) and R2 (consistency and higher melting points)

Reactions
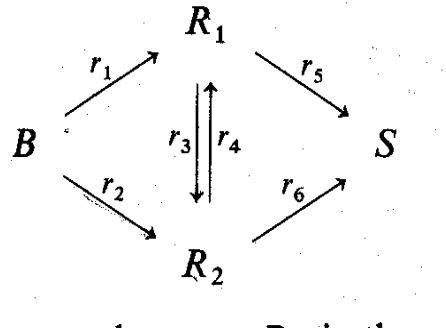
$$r_1 - r_4 \propto C_{H_2}^{1/2}, r_5 - r_6 \propto C_{H_2}$$

implies selectivity of monounsaturates over saturates proportional to $(C_{H_2})^{1/2}$

Yield conversion diagrams
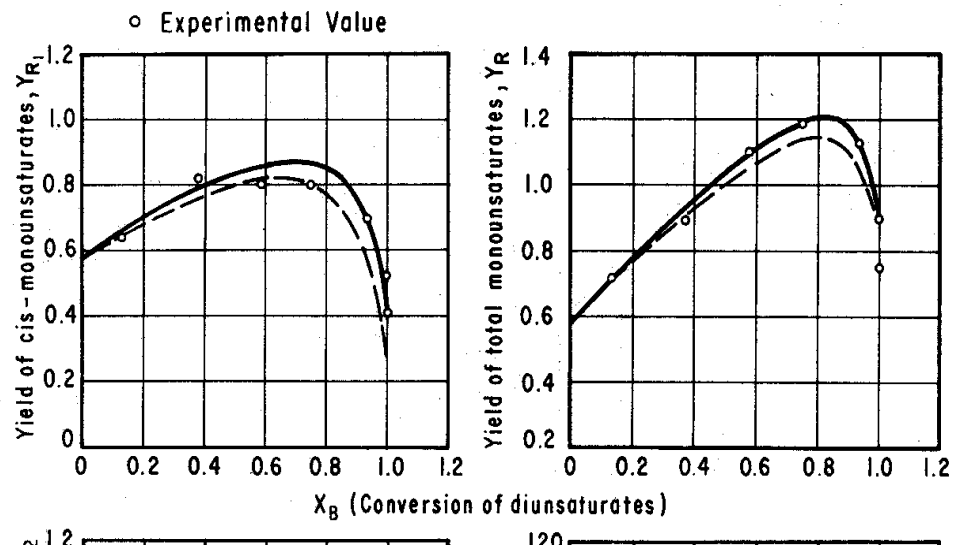
Balances

$$mass \quad \frac{dC_j}{dt} = R_j \quad j = B, R_1, R_2, M$$

$$-\overline{k_L} a_v \left(C_{H_2,g} - C_{H_2,s} \right) = R_{H_2} \left(C_j, C_{H_2,s} \right)$$

$$\frac{dC_{H_2,b}}{dt} = k_L a_v \left(C_{H_2,g} - C_{H_2,b} \right) - k_S a_S \left(C_{H_2,b} - C_{H_2,s} \right)$$

$$0 = k_S a_S \left(C_{H_2,b} - C_{H_2,s} \right) + R_{H_2}$$

$$\frac{1}{\overline{k_L} a_v} = \frac{1}{k_L a_v} + \frac{1}{k_S a_S}$$

Stirred tank batch reactor

Operating Liquid Height

Stagnant Liquid
Height (ungassed)

A

B   C
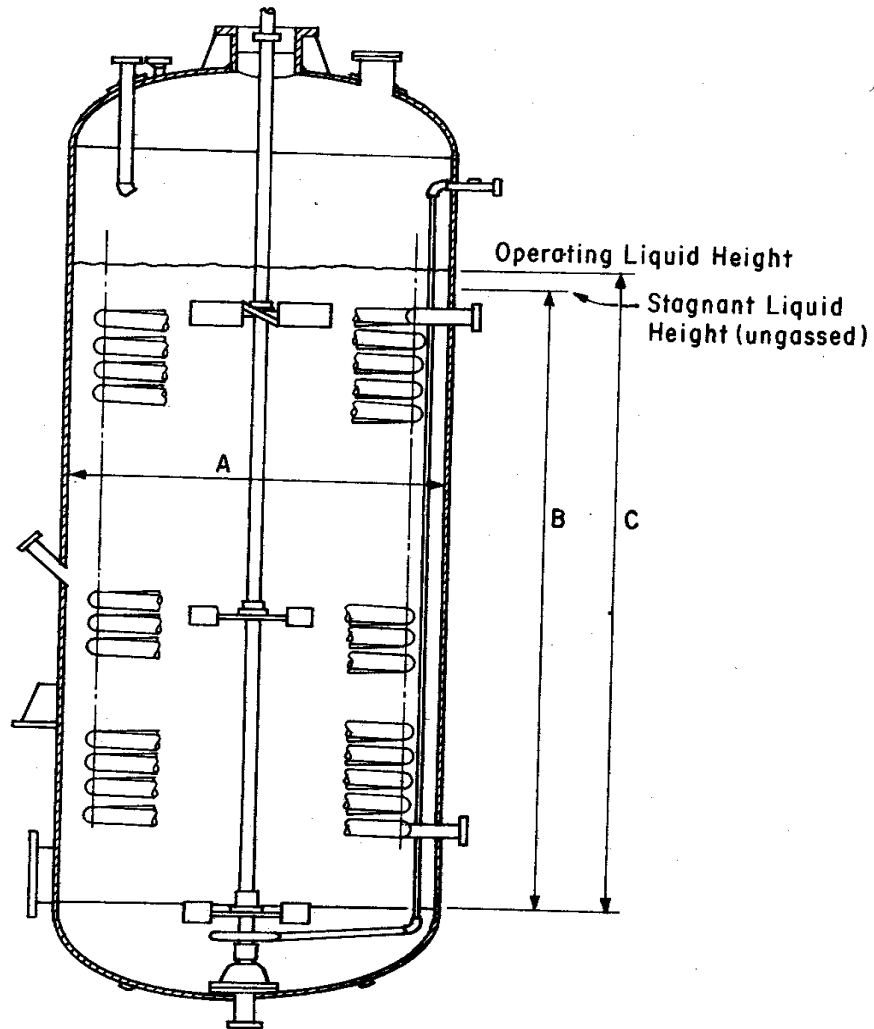
- Desired conversion – batch time

- Desired production rate and batch time – volume

- Based on volume – internal design

- Cooling load

$$-Q = V\sum_{i}(-\Delta H_i)r_i = A_K U(T - T_r)$$

Ammonia synthesis

- **Major demand – Fertilizer, chemicals, explosives, polyamides, pharmaceuticals; 150 million tons per annum**

- **Main reaction**

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightleftharpoons NH_3, \ \Delta H_{298K} = -45.7 \, kJ/mol^{-1}$$
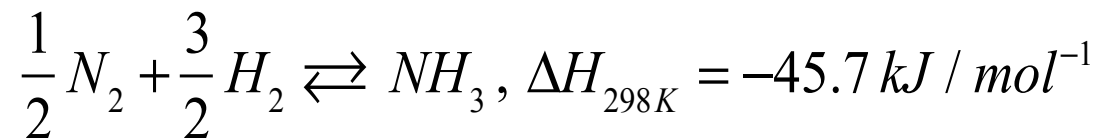
- **High pressure, low temperatures favorable**

- **Catalytic reaction – iron, promoted ruthenium**

Ammonia synthesis – equilibrium

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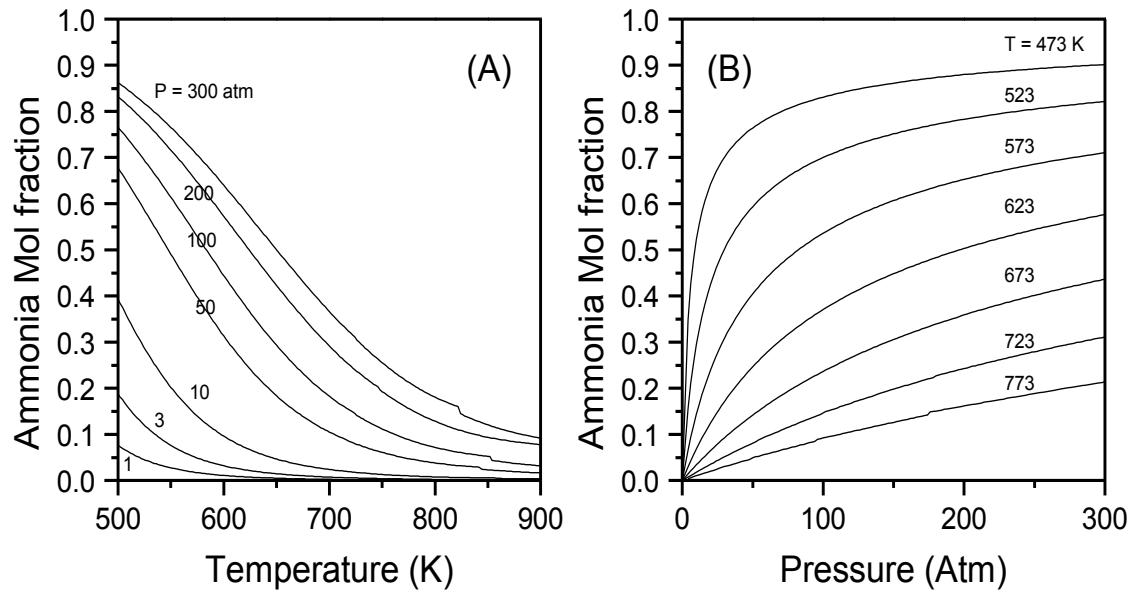
Ammonia synthesis - balances

mass

$$u_s \frac{dC_j}{dz} = \eta R_j \left(C_j, T \right)$$

energy

$$\rho_f u_s c_p \frac{dT}{dz} = \frac{4U}{d_t} \left(T_r - T \right) + \eta \left(-\Delta H \right) r$$

catalyst

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 D_{ie} \frac{dC_i'}{dr} \right) = -R_i \left(C_i', T' \right)$$

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \lambda_e \frac{dT'}{dr} \right) = \Delta H \, r$$

Reactor simulation
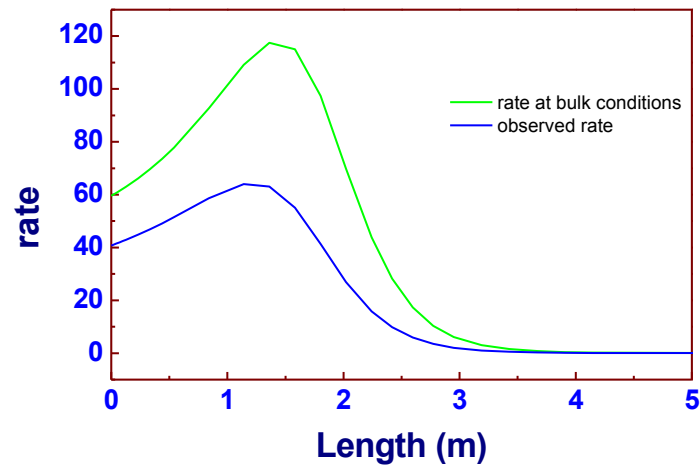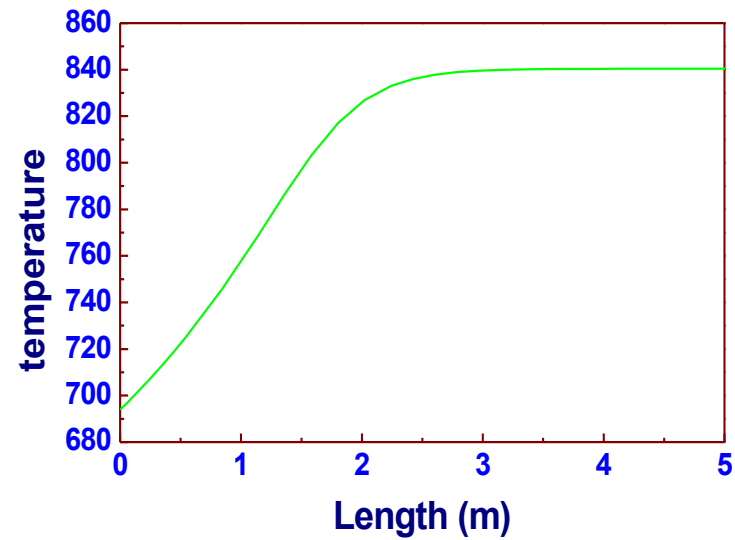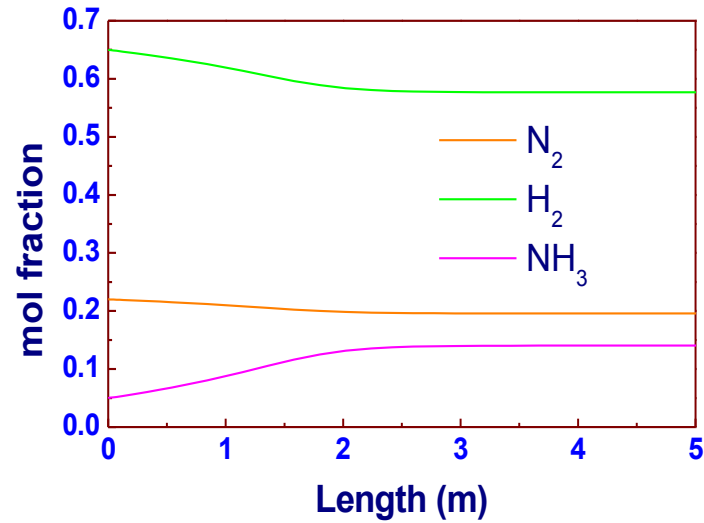
Optimal temperature

Fixed bed reactors

I, II, III, IV: Heaters
1, 2, 3, 4: Reactors
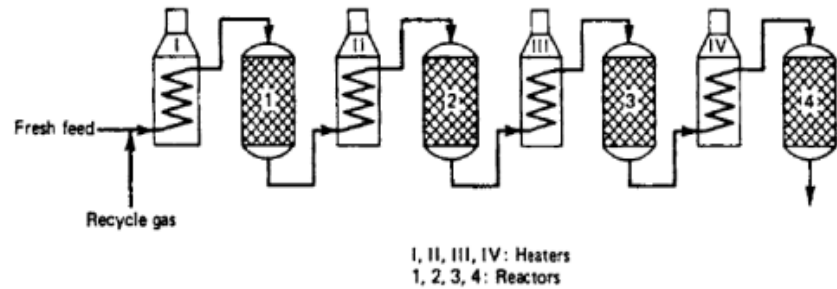
Figure 11.3-1 Multibed adiabatic reactor for catalytic reforming (from Smith [5]).
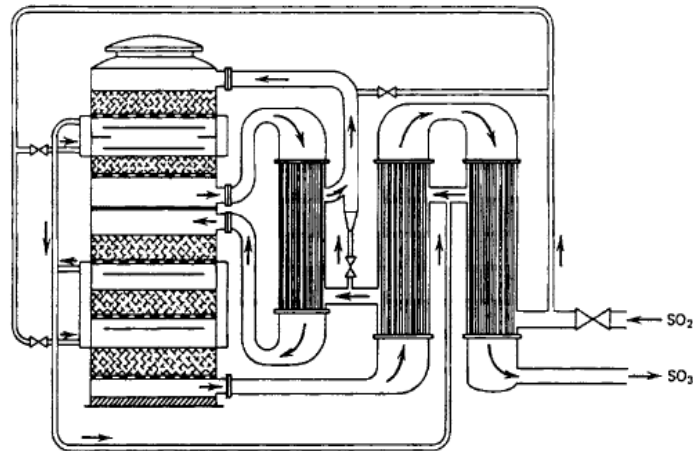
Figure 11.3-2 Multibed adiabatic reactor for SO₃ synthesis (after Winnacker and Kuechler [2], from Froment [148]).

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Ammonia – Multibed reactor
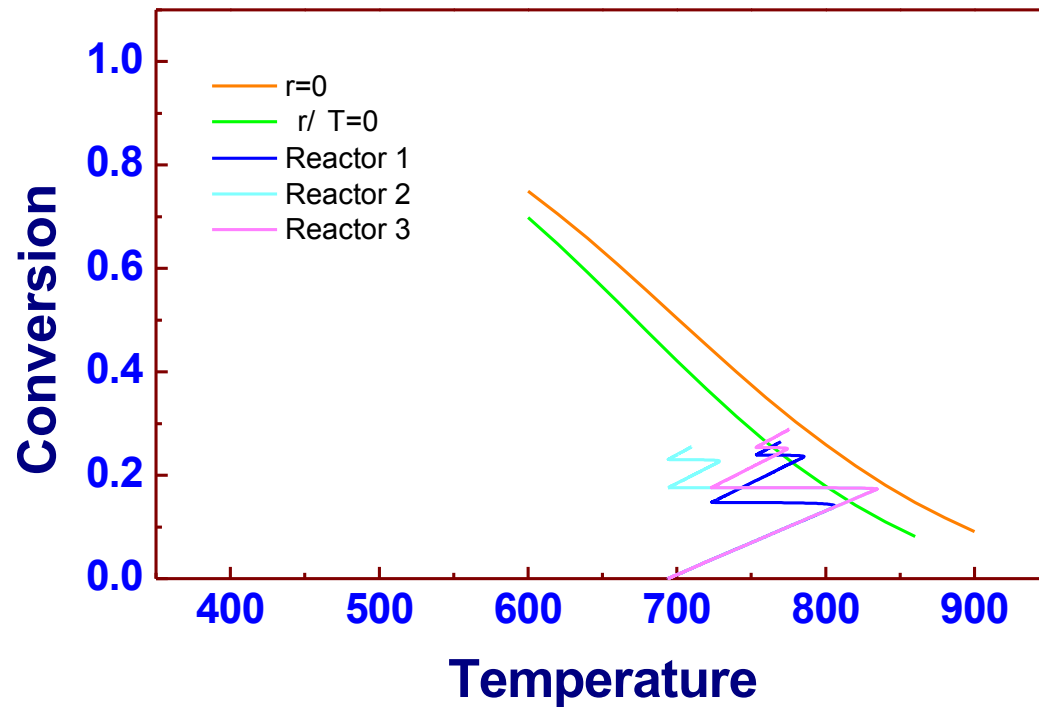
Fixed bed reactors
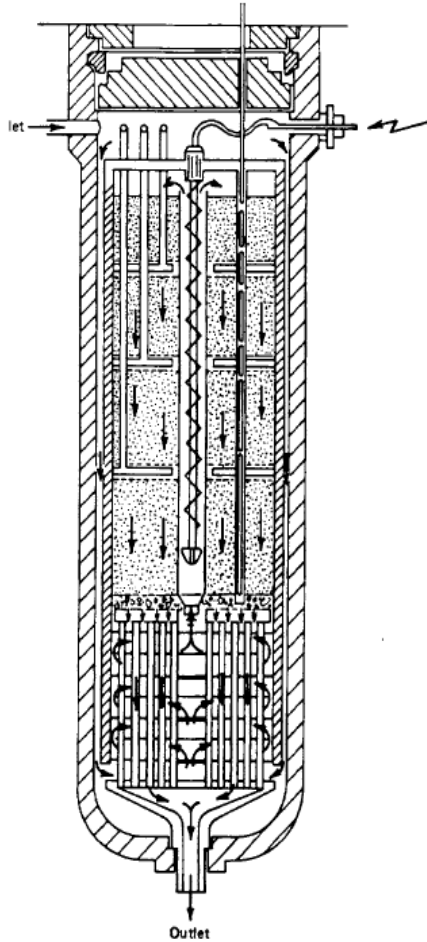
Figure 11.3-3 Multibed adiabatic reactor for NH₃ synthesis (after Winnacker and Kuechler [2], from Froment [148]).
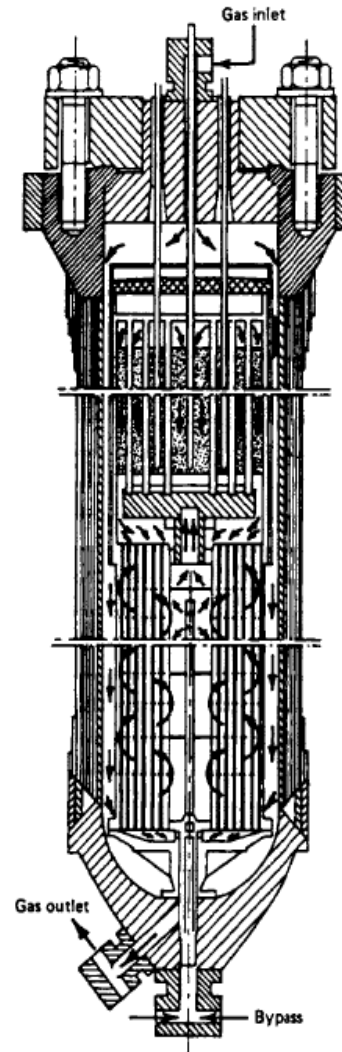
Figure 11.3-5 Ammonia synthesis reactor with tubular heat exchanger (from Vancini [4]).

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Ammonia – Autothermal

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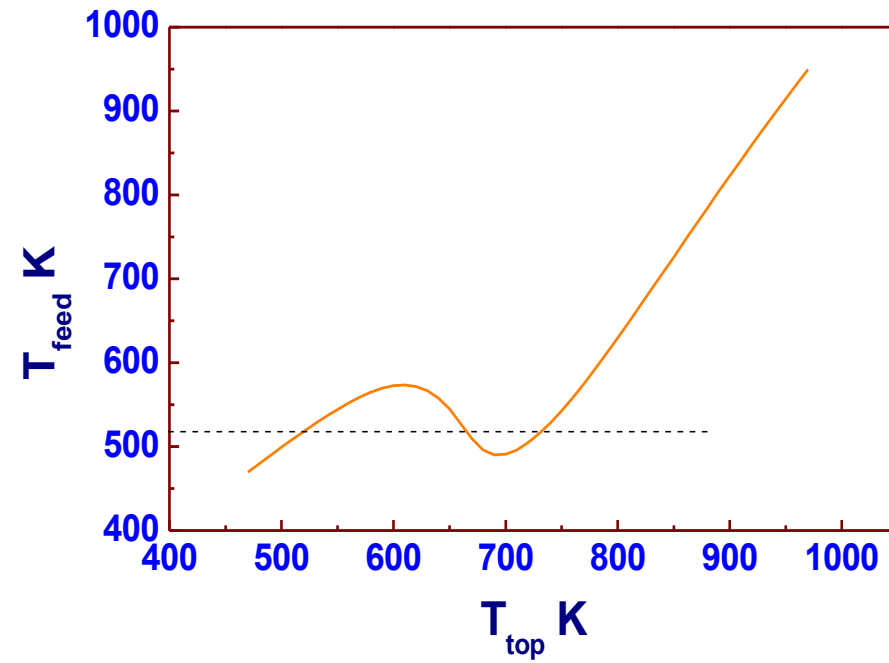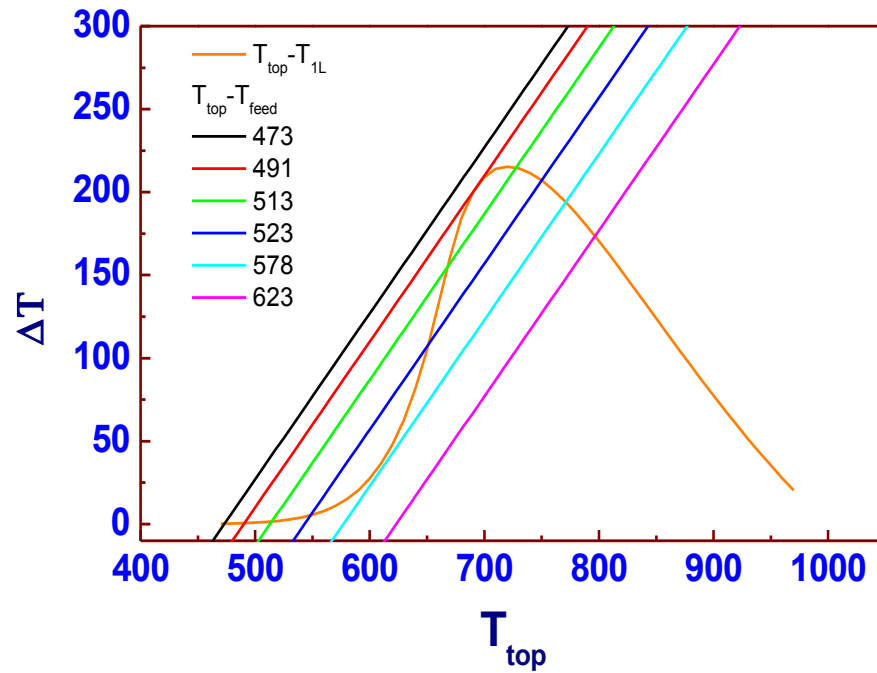
Ammonia – Autothermal
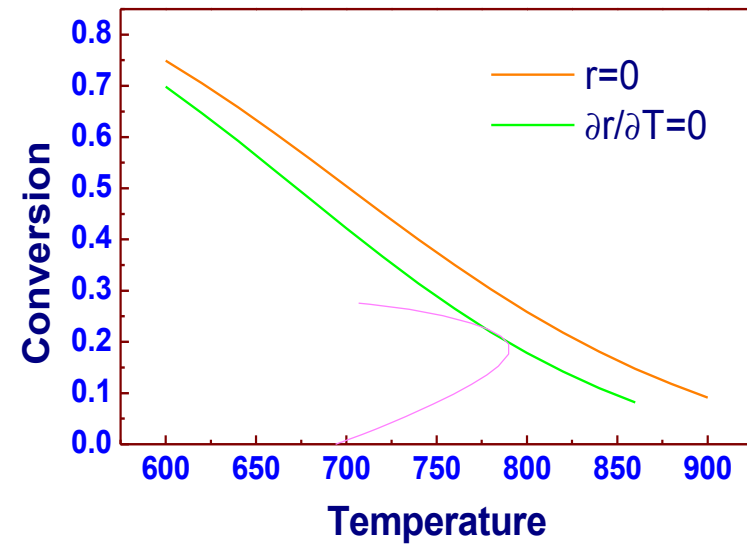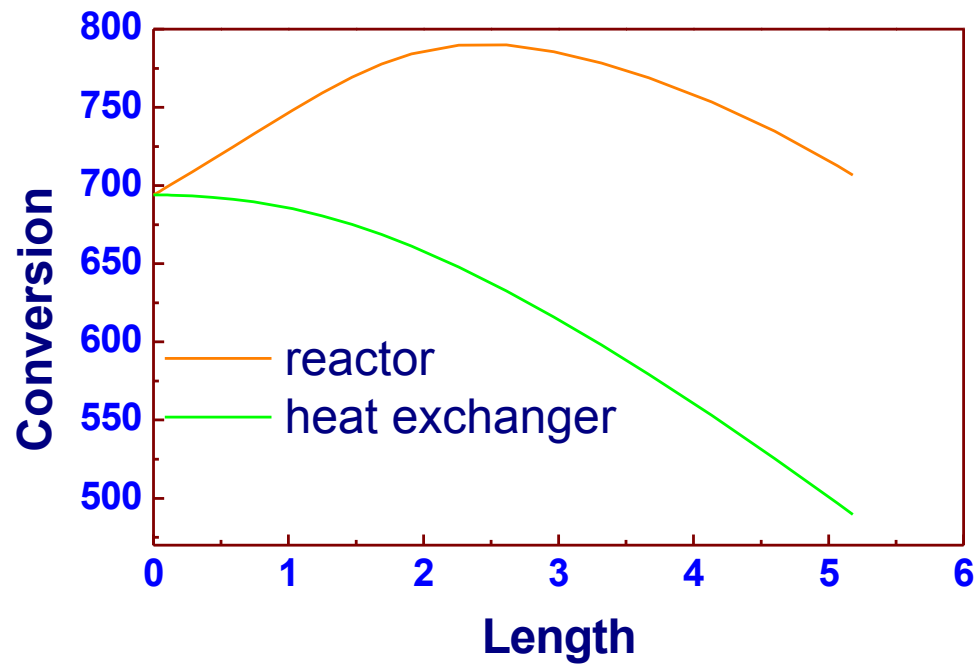
Process intensification

➢ Strategy of reduction in physical size of a chemical plant while achieving given objective

➢ 30 – 40 years old concept, reinvented in last decade due to intense competition, scarce resources and stricter environmental norms

➢ Multifunctional reactive systems – several functions are designed to occur simultaneously.

➢ Major drive in refining and petrochemicals sector

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Catalyst particle in reacting media
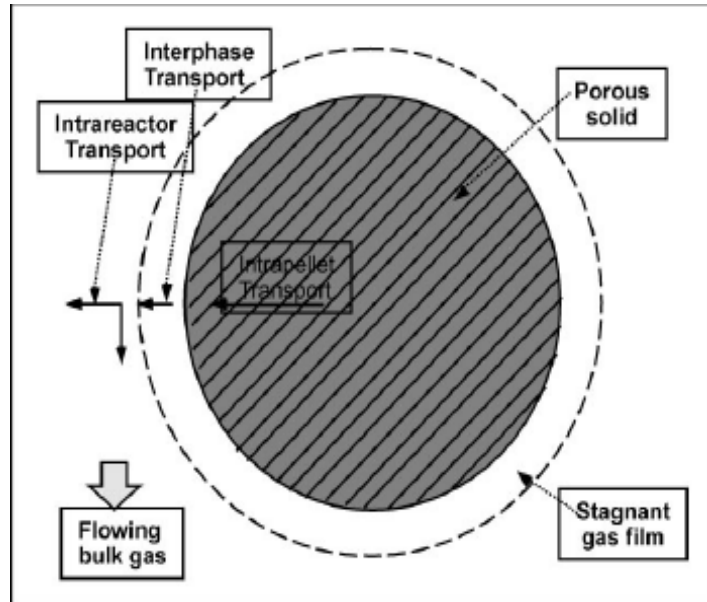
- Type A – at catalyst level
- Type B – at interphase transport level
- Type C – at intra-reactor level – separations/heat transfer
- Type D – inter-reactor level by combining two reactor operation with solids recirculation.

Type A Example – bifunctional catalysis

- ➢ Catalytic reforming to increase the octane number

- ➢ Conversion of parafins, cyclo parafins and napthenes to aromatics and branced paraffins.

- ➢ Reactions involved – dehydrogenation, cyclization and isomerization

- ➢ Pt/SiO$_2$ catalyst

Type B Example – Gas induction reactors

SHAFT

GAS SPACE

GAS BUBBLES

SOLIDS

SPARGER RING

DRAFT TUBE

STATOR
GASLIQUID
DISPERSION

GAS ENTRANCE

DRAFT TUBE

STATOR

GAS-LIQUID
DISPERSION

SELF INDUCING
IMPELLER

DISPERSING
IMPELLER

SUSPENDING
IMPELLER
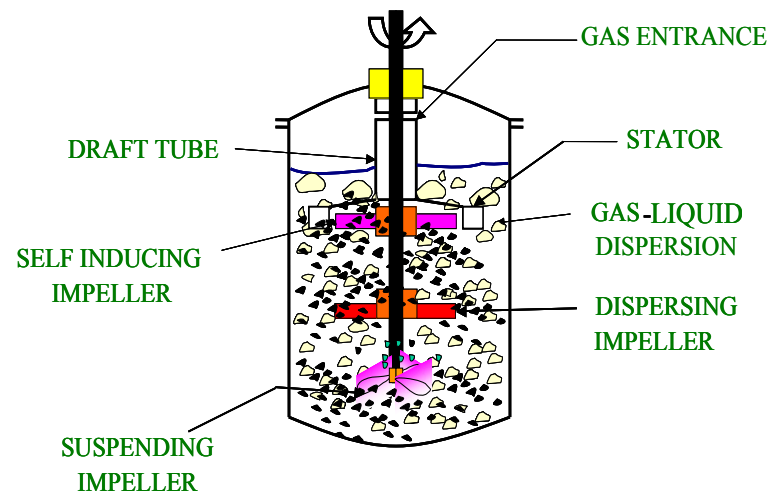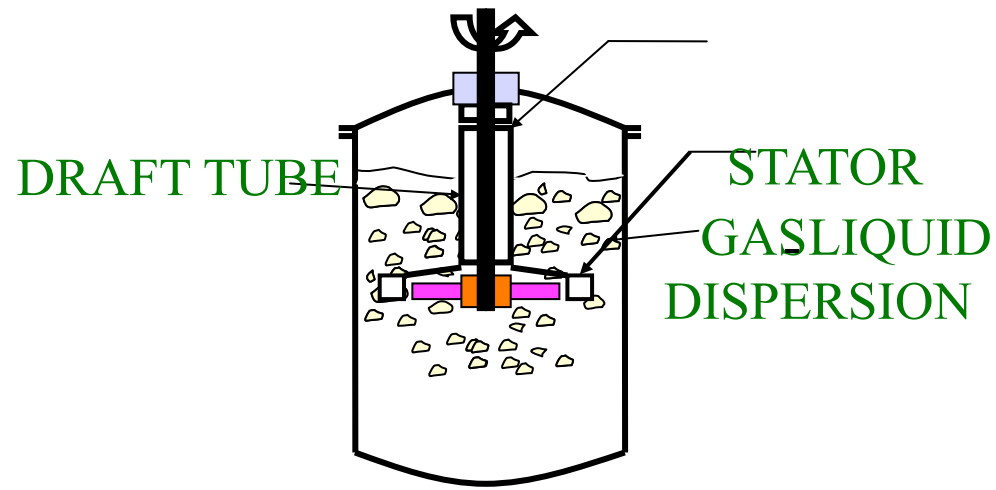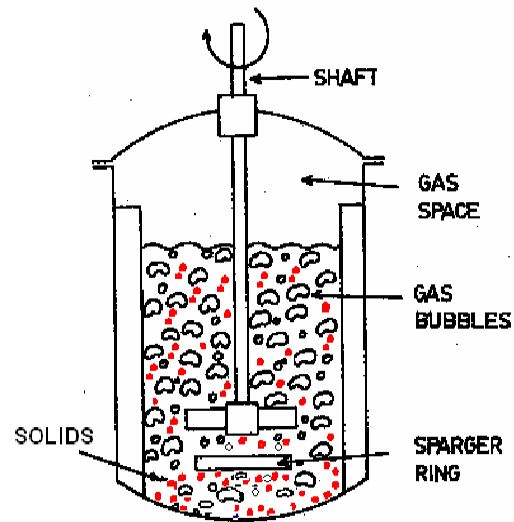
Type C – Intra-reactor operation

- ➢ Energy transfer – reaction in heat exchanger
- ➢ Momentum transfer – radial flow reactors
- ➢ Mass transfer – reactive- distillation, absorption

Type C – Momentum transfer

➢ **High gas flow rates – ammonia synthesis, styrene from ethylbenzene, flue gas treatments**
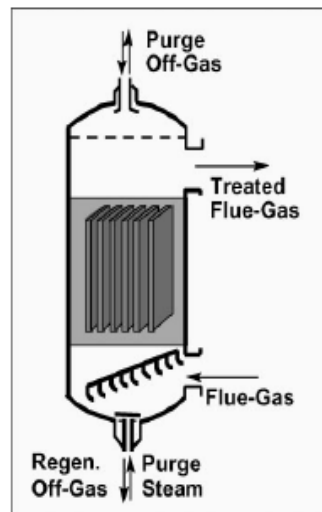
Parallel Passage Reactor
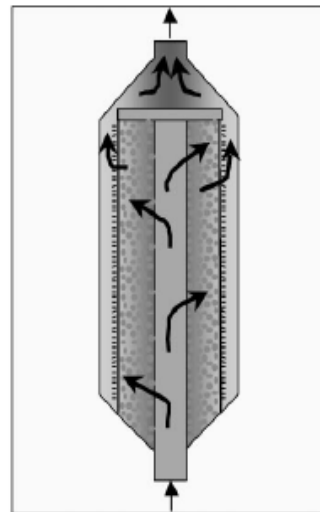
Radial Flow Reactor
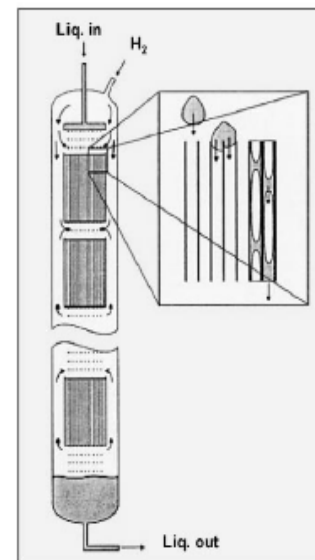
Monolith Reactor

Type C – Mass transfer

➢ **Enhance conversion in equilibrium limited reaction, prevent undesirable reaction, increase rate of product inhibited reactions**

Type C – Energy transfer

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \qquad \Delta H = 206 \ kJ/mol$$

$$CH_4 + 2O_2 \rightleftharpoons CO_2 + 2H_2O \qquad \Delta H = -803 \ kJ/mol$$
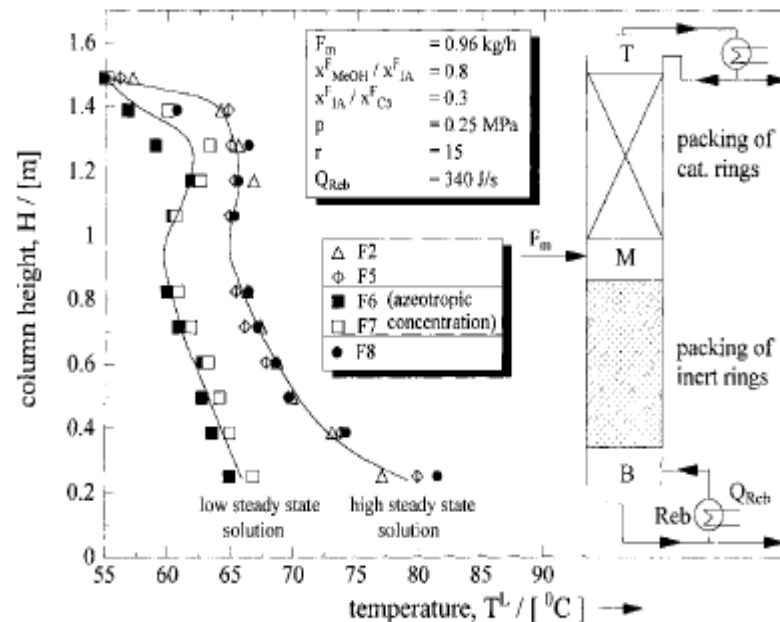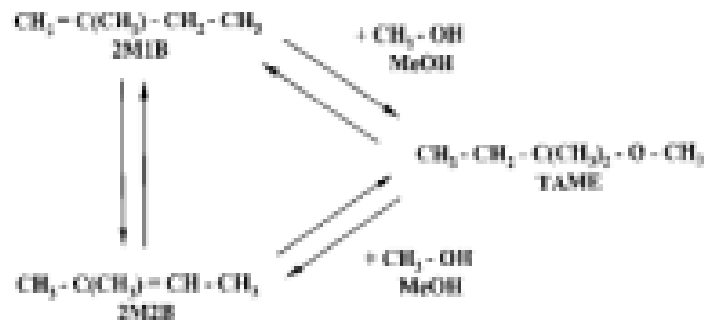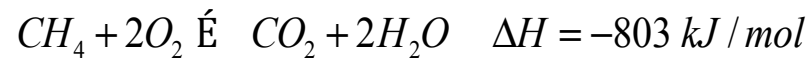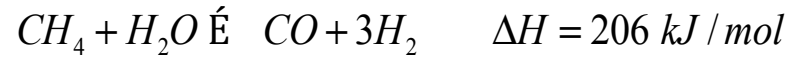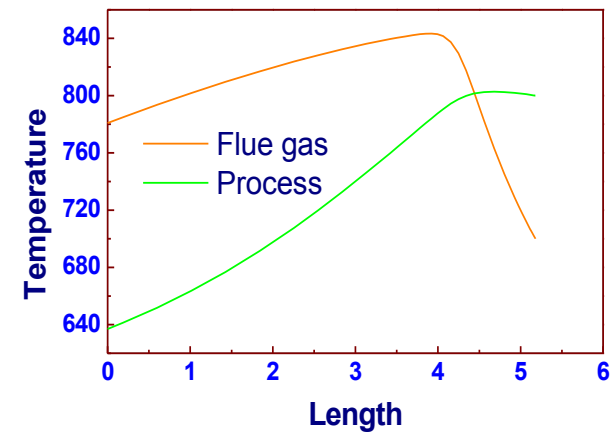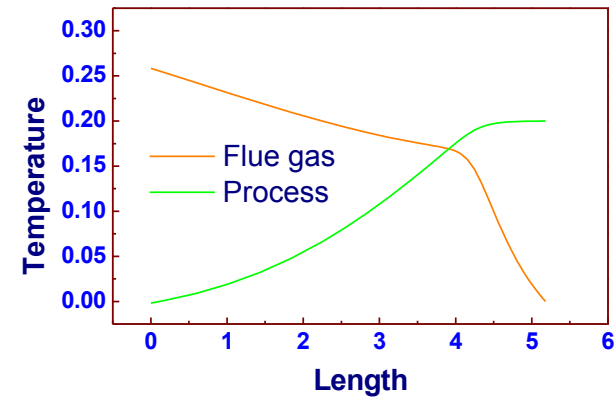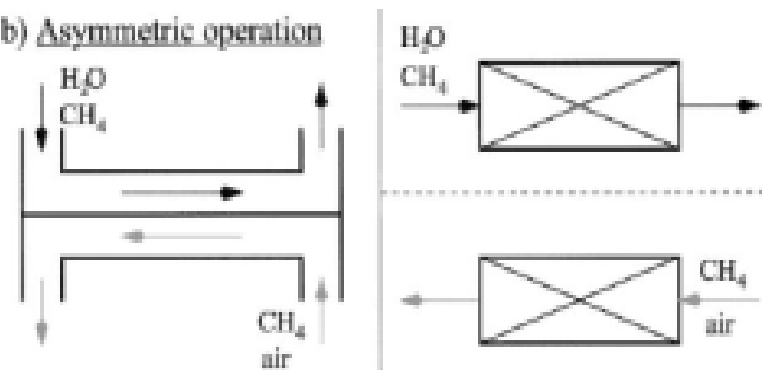
Type C – Example styrene synthesis
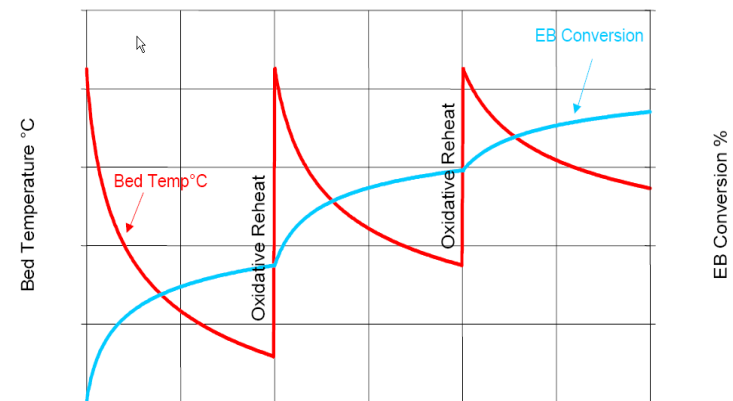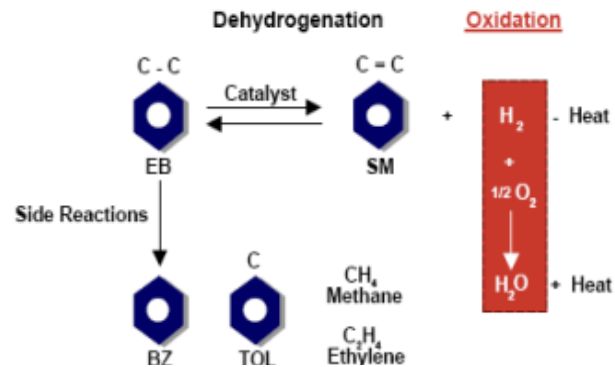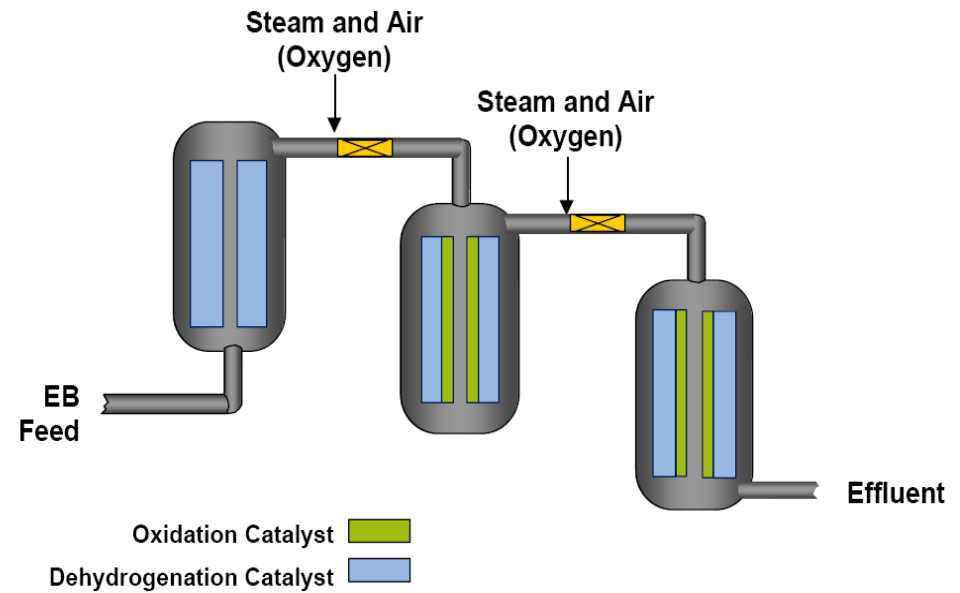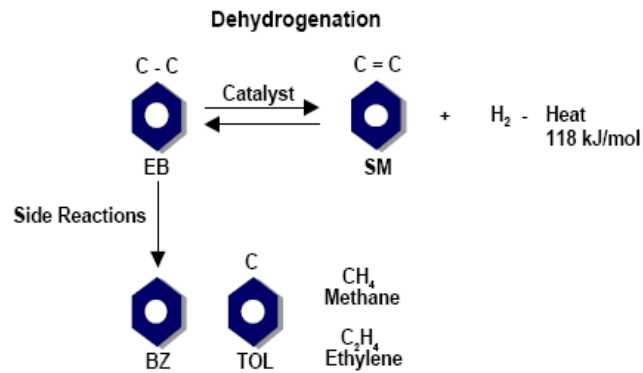
Design considerations and safety

Multiplicity in stirred tank reactor
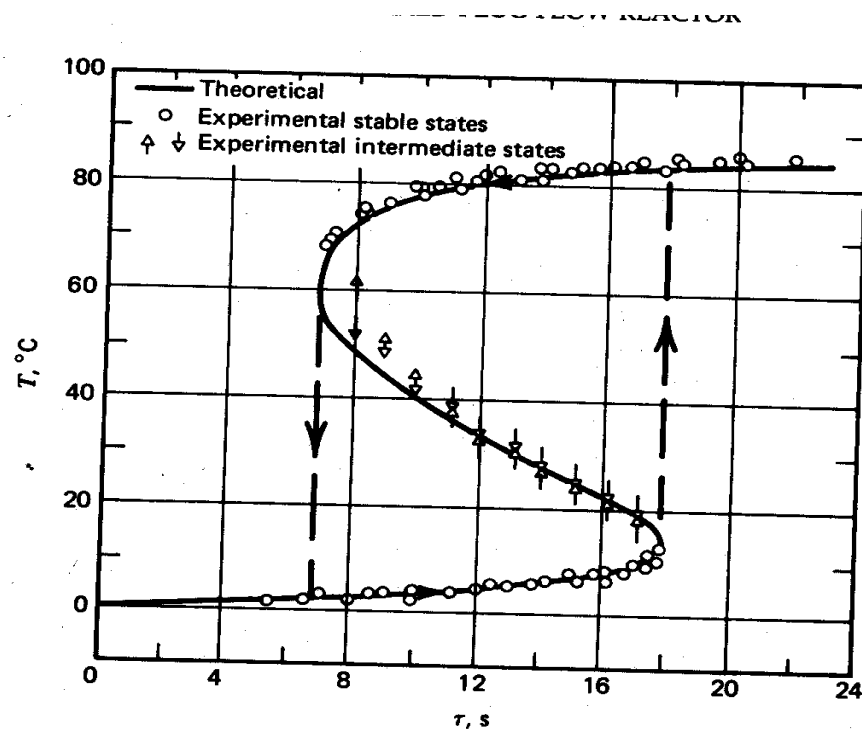
Figure 10.4.1-4
Steady-state hysteresis results. From Vejtassa and Schmitz (1970).
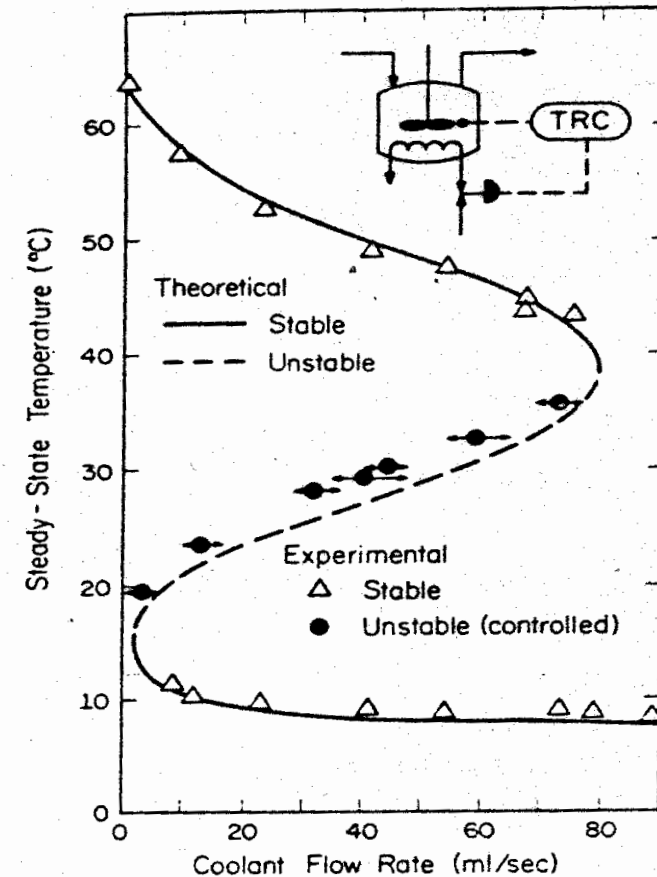
Explosion in batch reactor
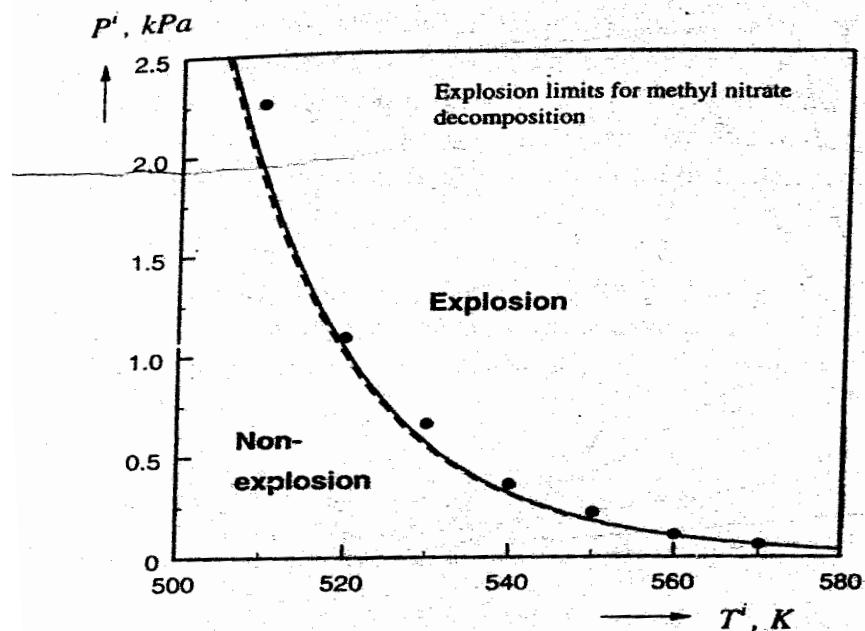
Figure 3.3. Explosion limits for methyl nitrate decomposition as measured experimentally by Gray *et al.* (1981) (●) and predicted by Semenov criteria in the form of Eqs. (3.16) and (3.18) (solid curve) or Eq. (3.21) (broken curve).
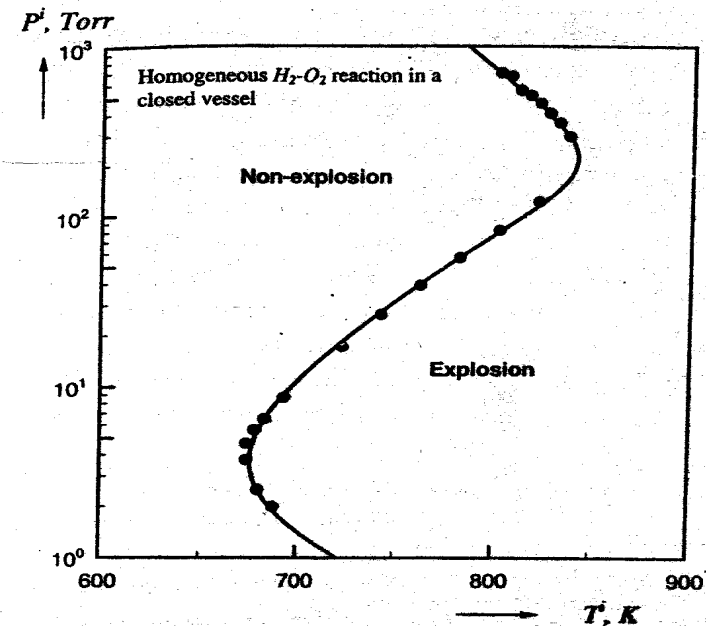
Figure 1.4. Stoichiometric H_2–O_2 mixtures in a closed vessel. The boundary representing the sensitive region in the initial pressure-initial temperature plane, which separates the non-explosion from explosion regions, measured experimentally by Lewis and von Elbe (1961).

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Runaway/Hot spot in tubular reactor
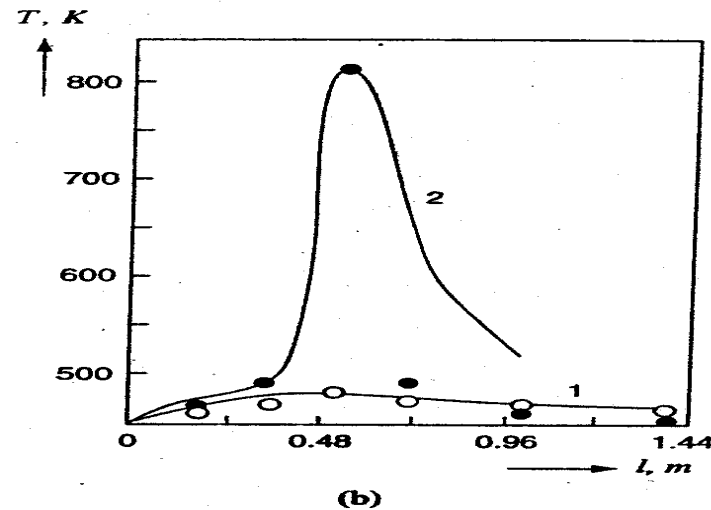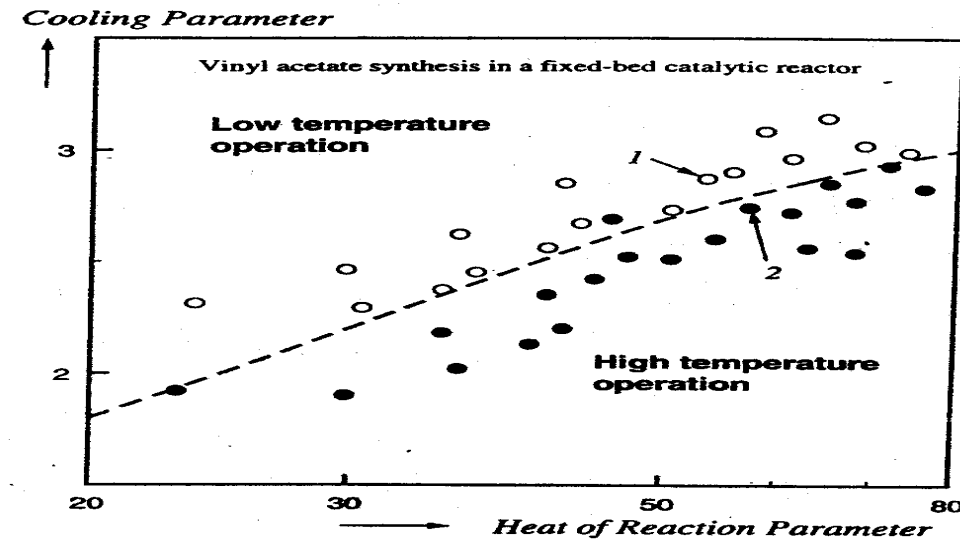
Figure 1.3. Vinyl acetate synthesis in a fixed-bed catalytic reactor. (a) Sensitive operation region in the cooling versus heat of reaction parameter plane, measured experimentally by Emig *et al.* (1980), where o = low temperature operation and • = high temperature operation. (b) Temperature profiles along the reactor length corresponding to the two operation conditions indicated by points *1* and *2* in (a).

Runaway/Hot spot in tubular reactor
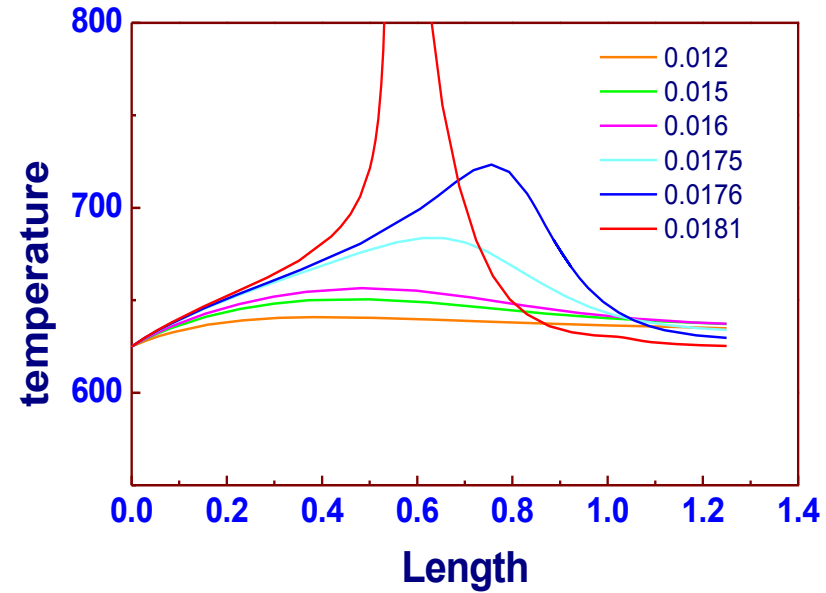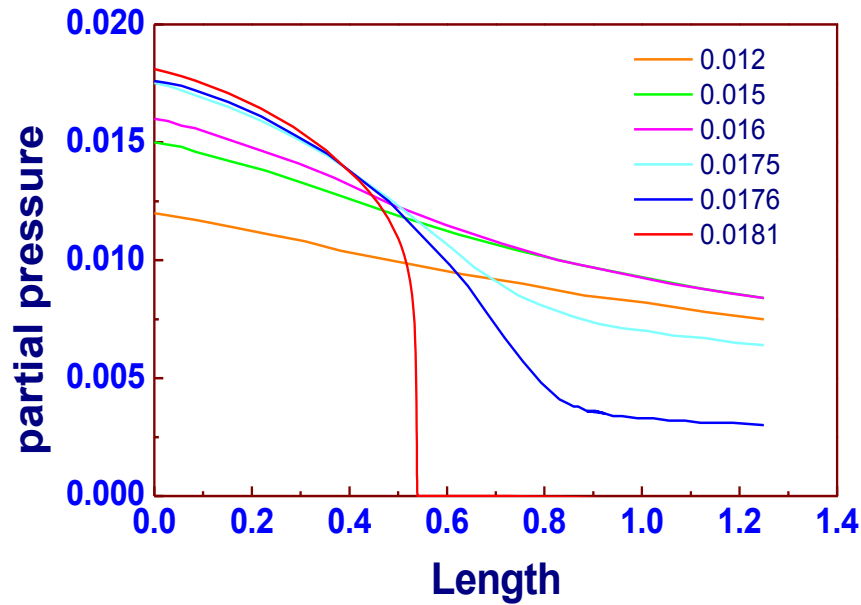
Runaway/Hotspot in tubular reactors
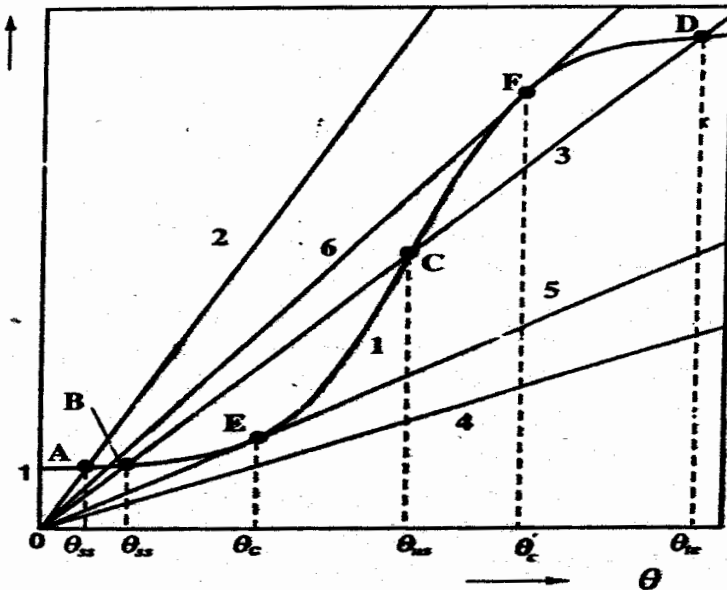
Figure 3.1. Temperature-increase rate θ_+ (curve 1) and temperature-decrease rate θ_- (curves 2 to 6) as functions of the system temperature θ: an illustration of the Semenov theory of thermal explosion.

stable node

$q < p^2/4$
$\lambda_{1,2} = \alpha_1, \alpha_2$
'α' < 0

stable spiral

unstable spiral

unstable node

$q < p^2/4$
$\lambda_{1,2} = \alpha_1, \alpha_2$
$\alpha_1 > 0, \alpha_1 > \alpha_2$

$q < p^2/4$
$\lambda_{1,2} = \alpha_1, \alpha_2 > 0$

$p = \text{tr}(A)$

saddle

unstable manifold

stable manifold
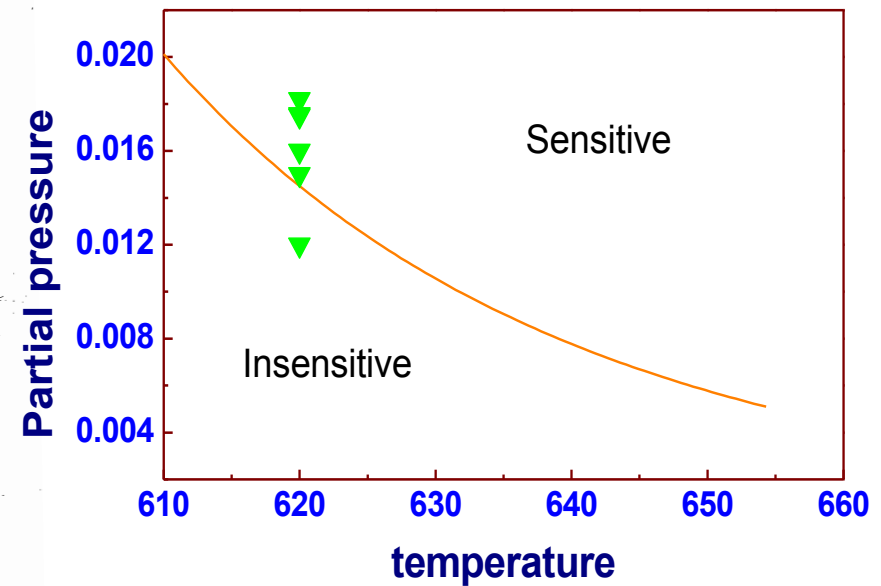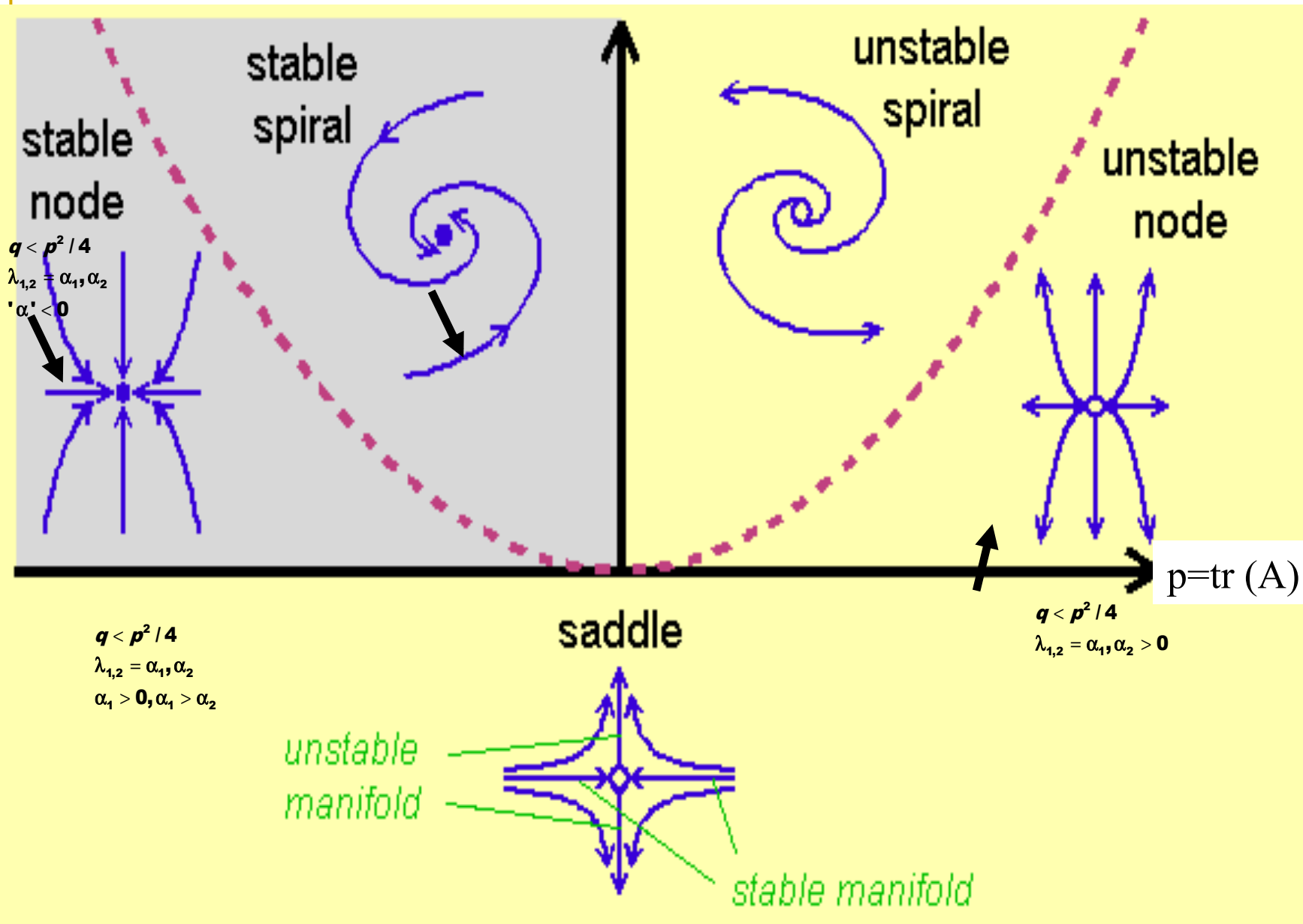
Stability analysis

➢ A state X=0 is said to be stable when given e>0, there exists a d>0 (0<d<e) such that if ||X(0)||<d then ||X(t)|| < e for all t>0

➢ A state X=0 is said to be asymptotically attractive when given m>0, such that if ||X(0)|| <m then lim (t→∞) ||X(t)|| =0

➢ A state is asymptotically stable when stable and asymptotically attractive.

➢ A state is marginally stable when stable but not asymptotically attractive

Examples

$$\frac{dx}{dt} = \frac{x^2(y-x)+y^5}{1+x^2+y^2+(x^2+y^2)^2}$$

$$\frac{dy}{dt} = \frac{y^2(y-2x)}{1+x^2+y^2+(x^2+y^2)^2}$$

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = -x$$
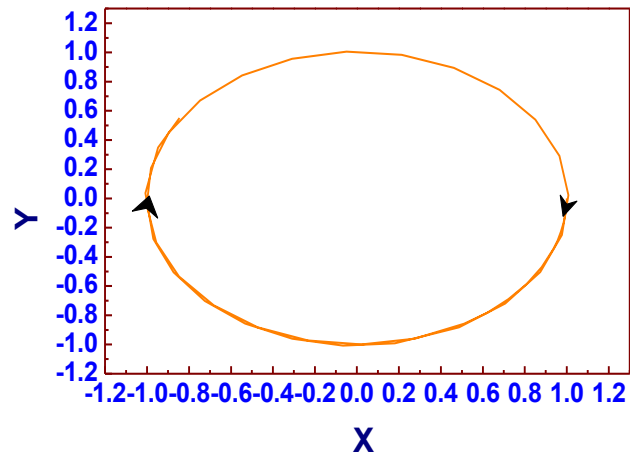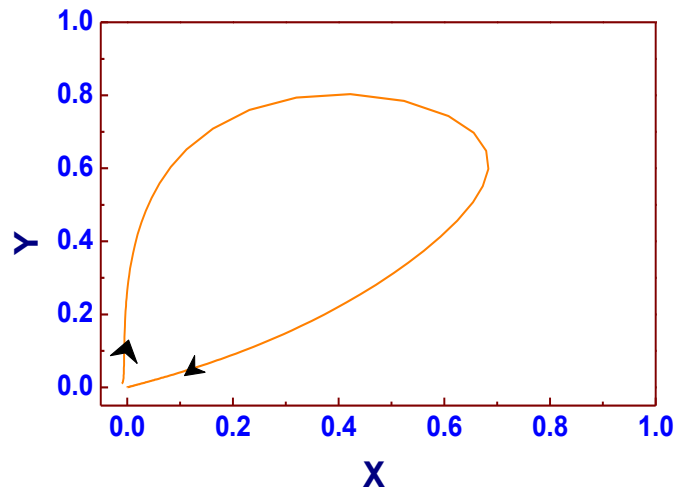
Two dimensional system - Eigen values

$$\lambda^2 - T\lambda + D = 0 \qquad \Rightarrow \lambda_{1,2} = \frac{T}{2} \pm \sqrt{\frac{T^2}{4} - D}$$
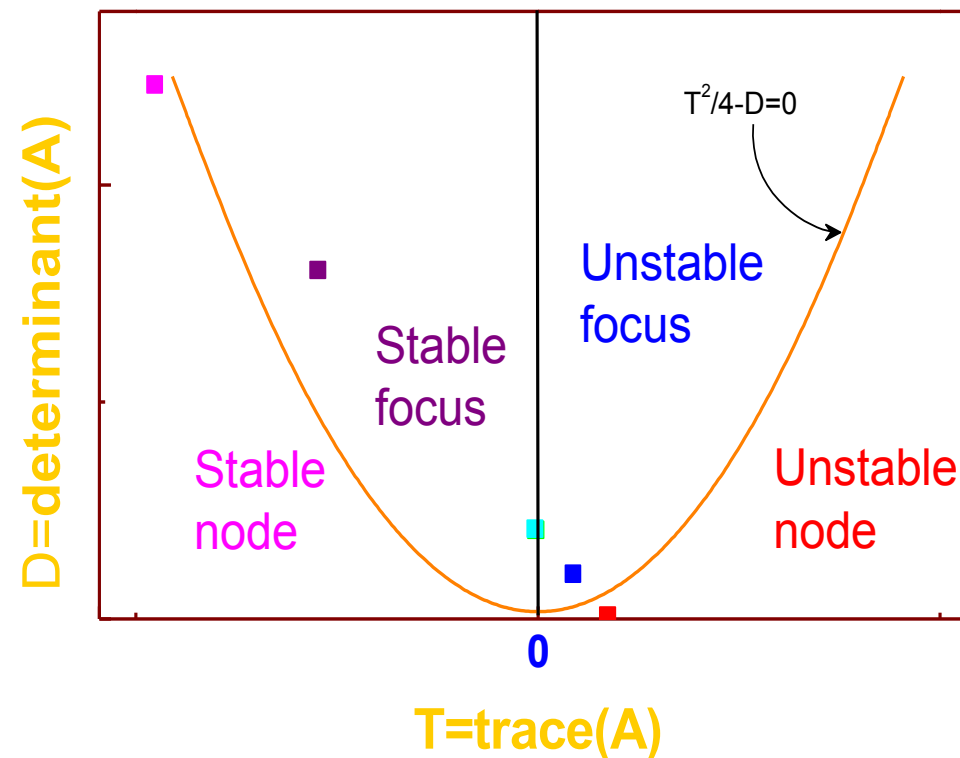
Unstable node

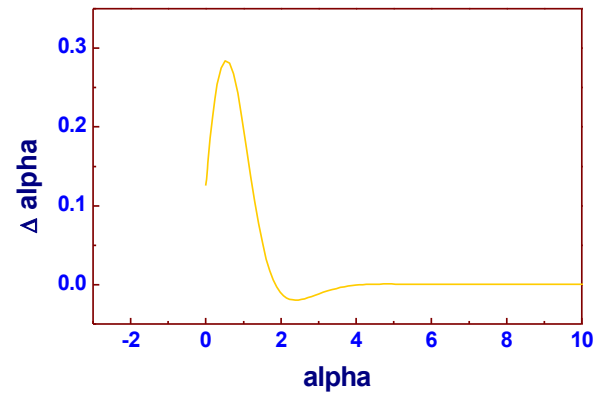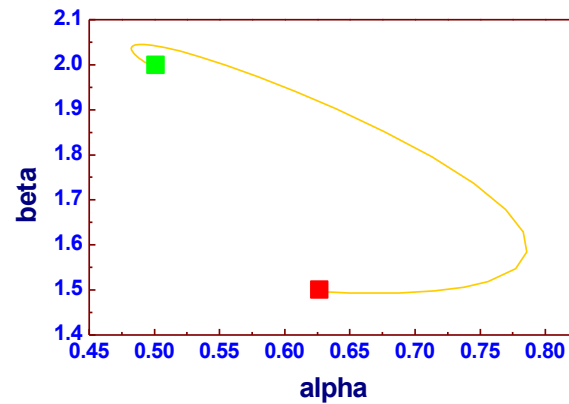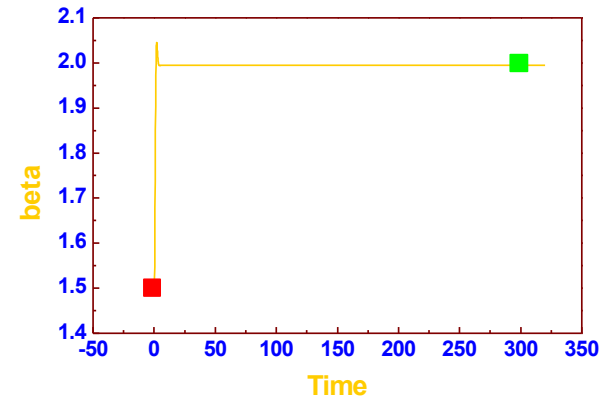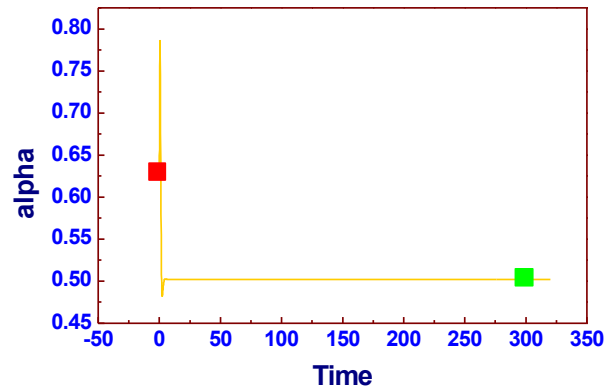$$\mu = 0.1 \quad D = 0.00971, \ T = 0.988 \qquad \lambda = 0.0099, 0.9782$$
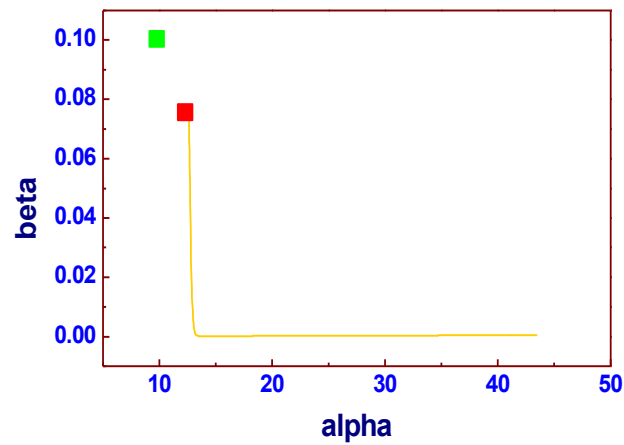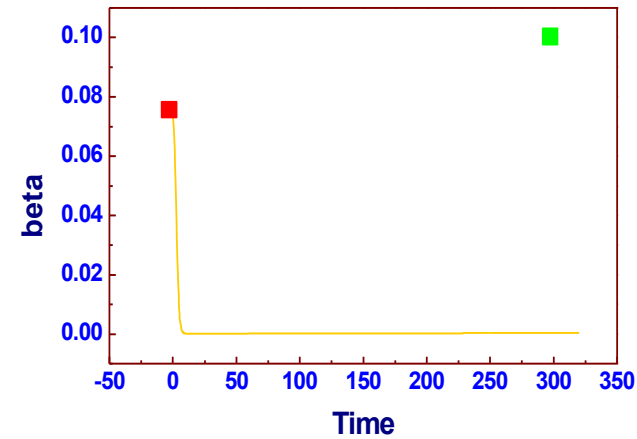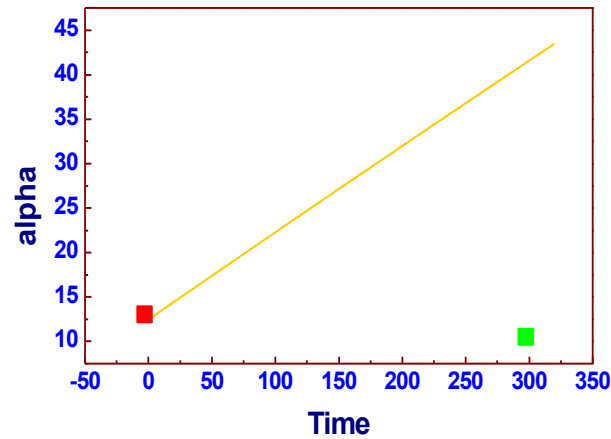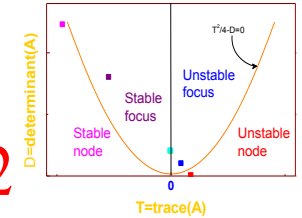
Unstable focus

$$\mu = 0.5 \quad D = 0.248, \; T = 0.751 \qquad \lambda = \boldsymbol{0.3756 \; \pm \; 0.3276i}$$

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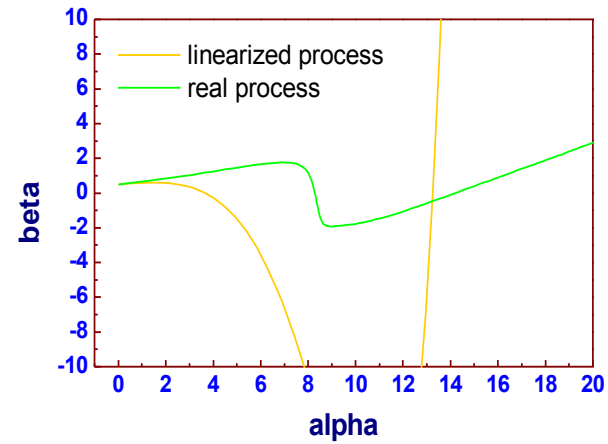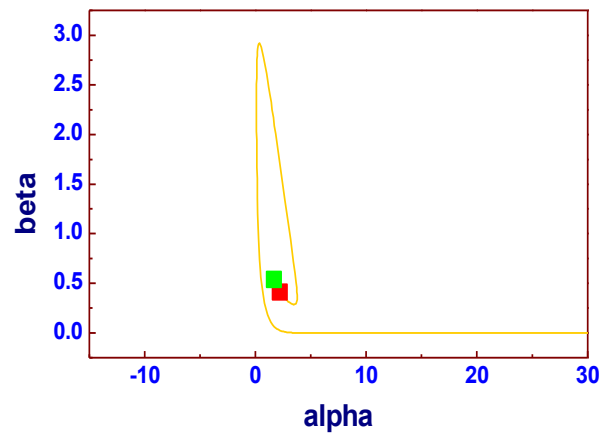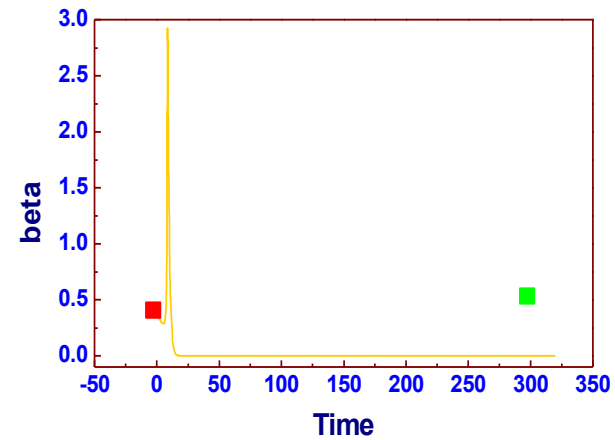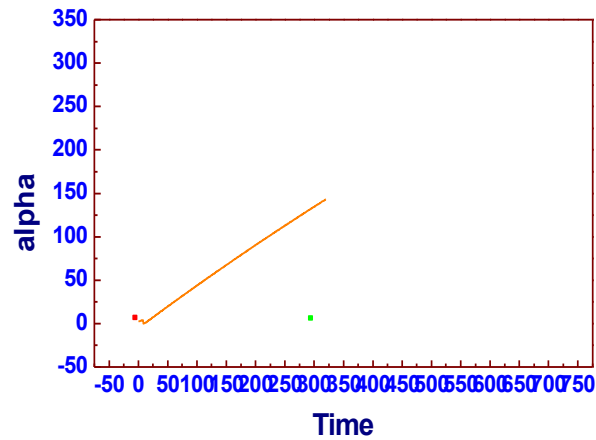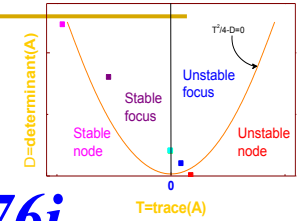
Stable focus

$$\mu = 2.0 \quad D = 3.99, \ T = -2.98 \ \lambda = \textbf{\textit{-1.4900}} \pm \textbf{\textit{1.3288i}}$$
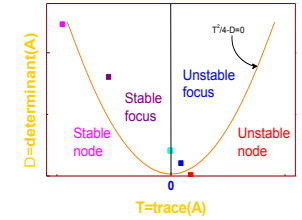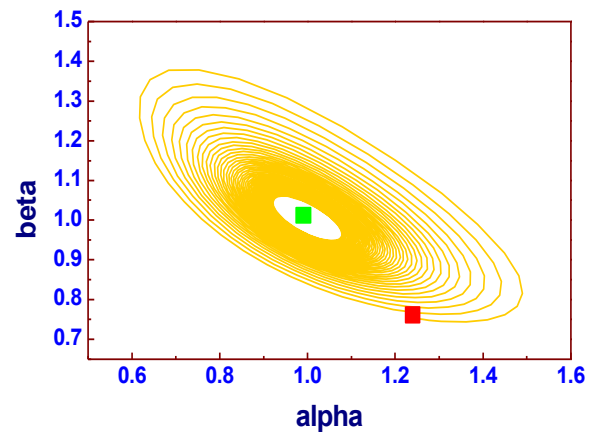
Stable node
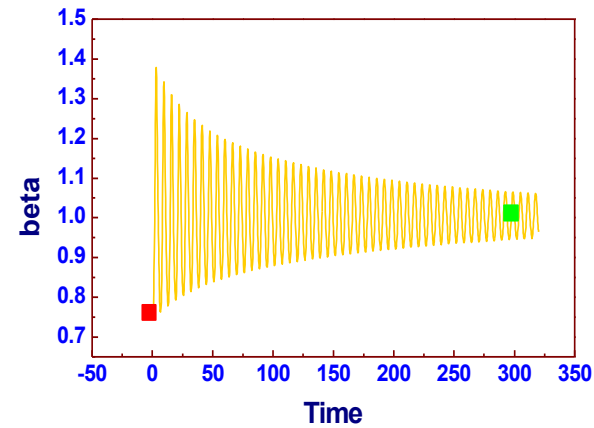
$\mu = 2.5$ $D = 6.23, T = -5.21$ $\lambda = -3.3614, -1.8525$
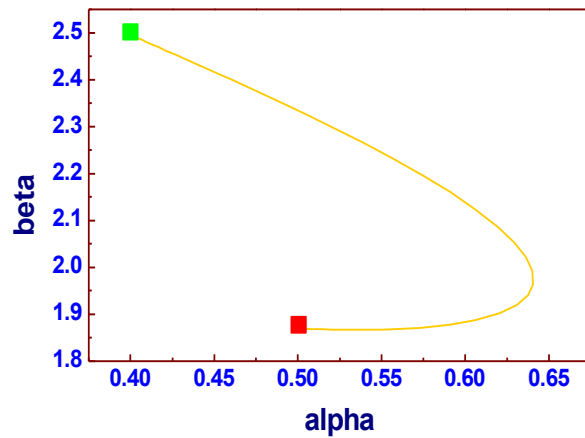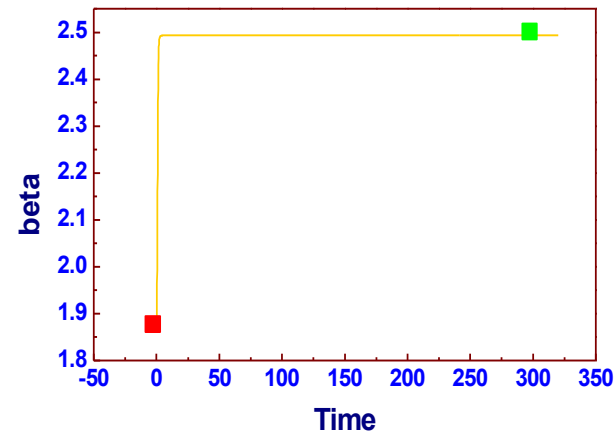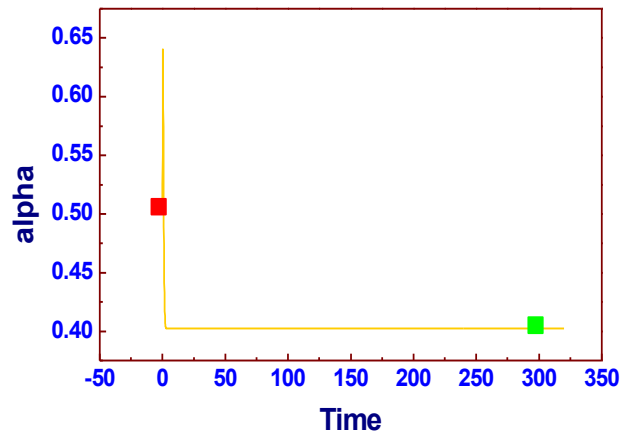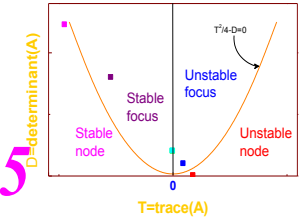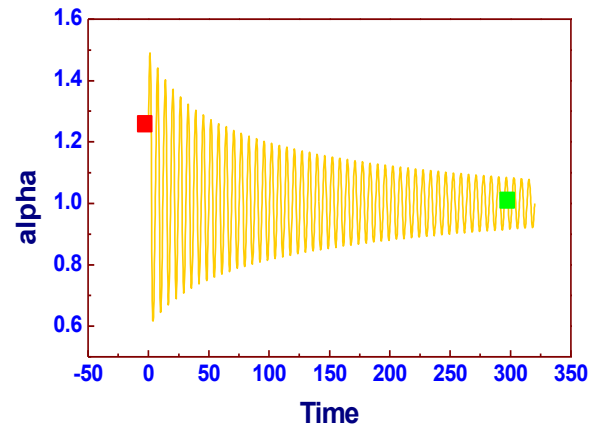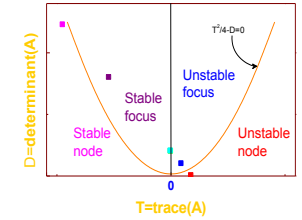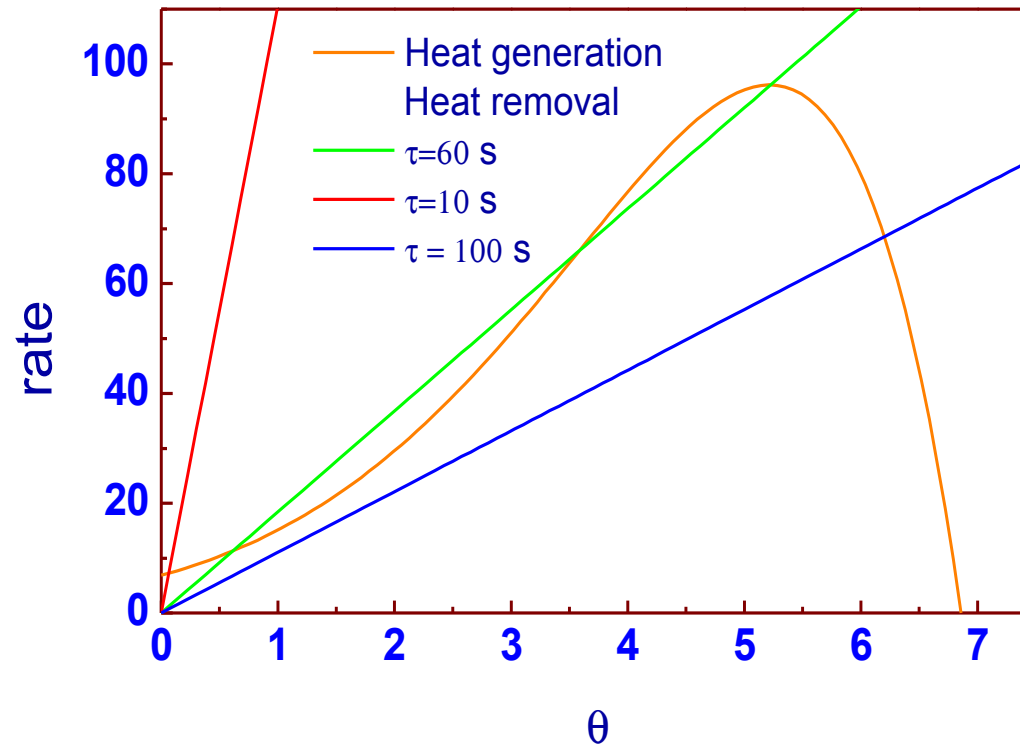
Limit cycle

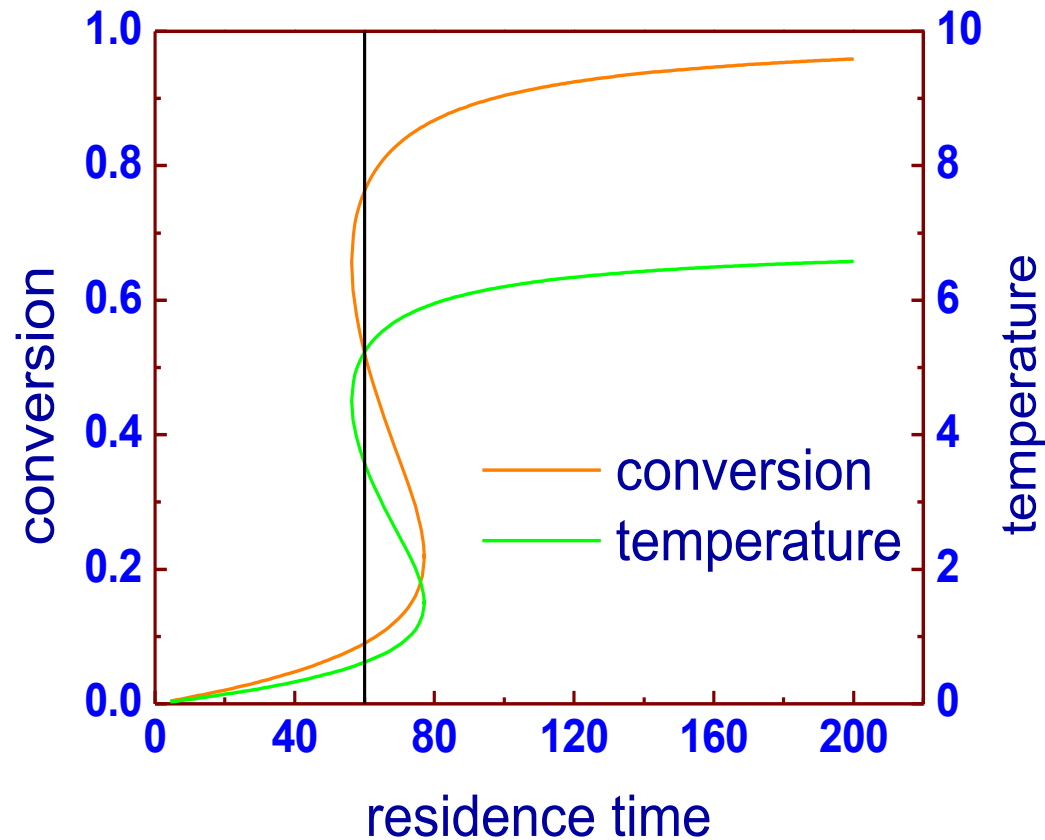$$\mu = 1.005 \qquad D = 1.01, T = 0 \qquad \lambda = \pm 1.003i$$
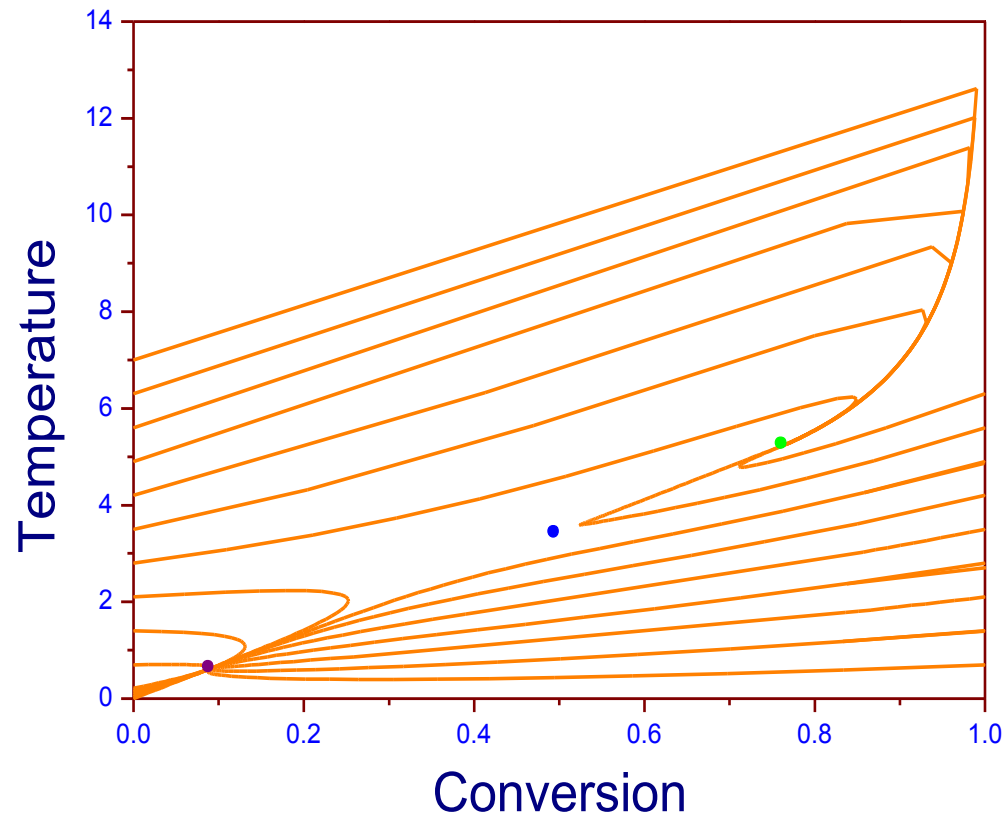
Adiabatic CSTR

Adiabatic CSTR – steady state multiplicity

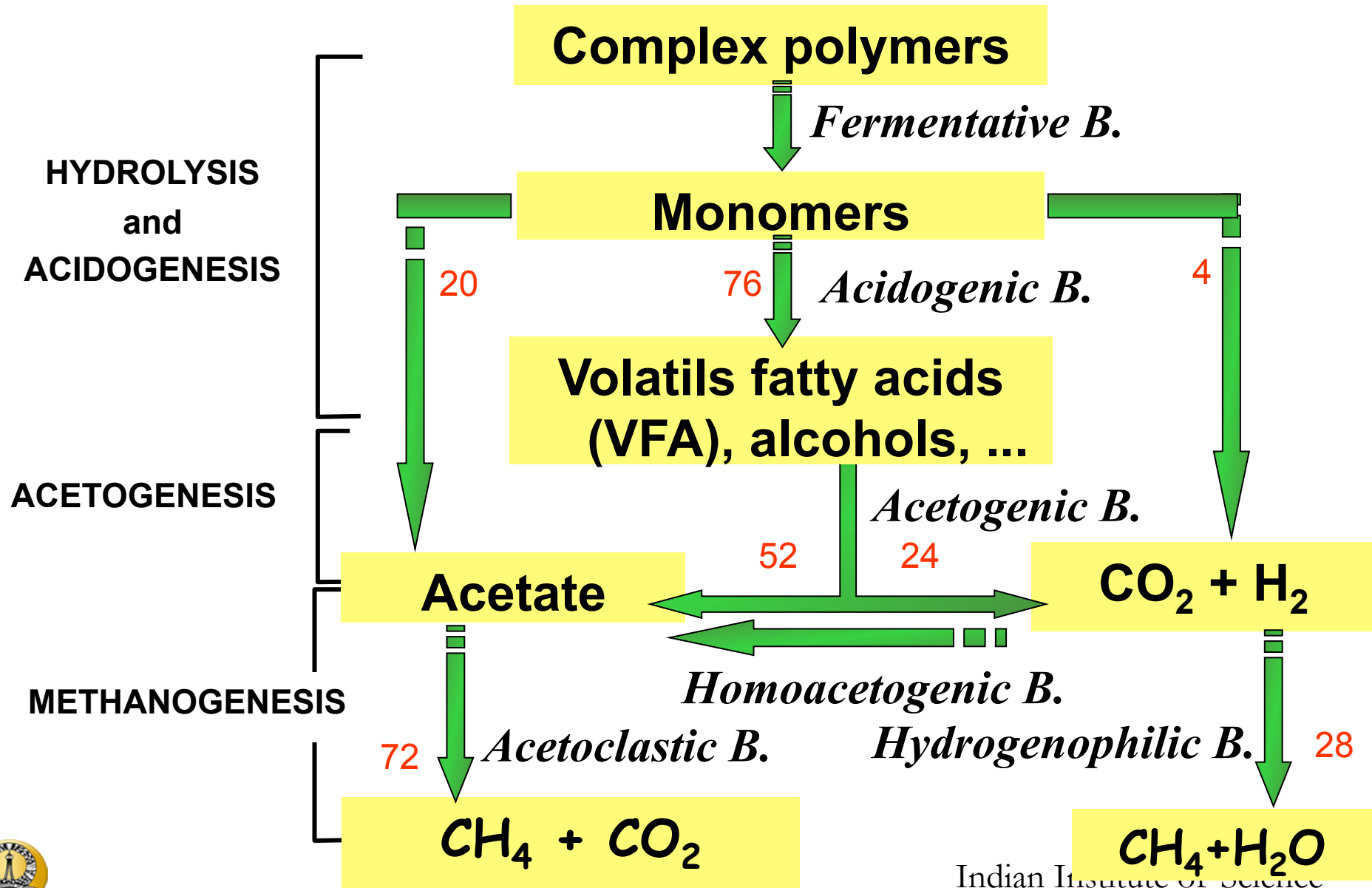| Steady state	Eigenvalues
0.08996, 0.61698	-1.67×10^{-2} , -8.68×10^{-3}
0.4957 3.4	-1.67×10^{-2} 7.05×10^{-3}
0.7628 5.2318	-1.74×10^{-2} -1.66×10^{-2}

Adiabatic CSTR – phase plane, transient

Non-ideal flow, mixing and reactions

➢ If, we know precisely what is happening within the vessel, thus, if we have a complete velocity distribution map for the fluid in the vessel, then we should, in principle, be able to predict the behavior of a vessel as a reactor. Unfortunately, this approach is impractical, even in today's computer age. *Levenspiel, Chemical Reaction Engineering, 1999.*

➢ Mobil Adds Million-Dollar Benefits by Using Flow Simulation to Optimize Refinery Units*, Greg Muldowney, Mobil Technology Company, 2007*
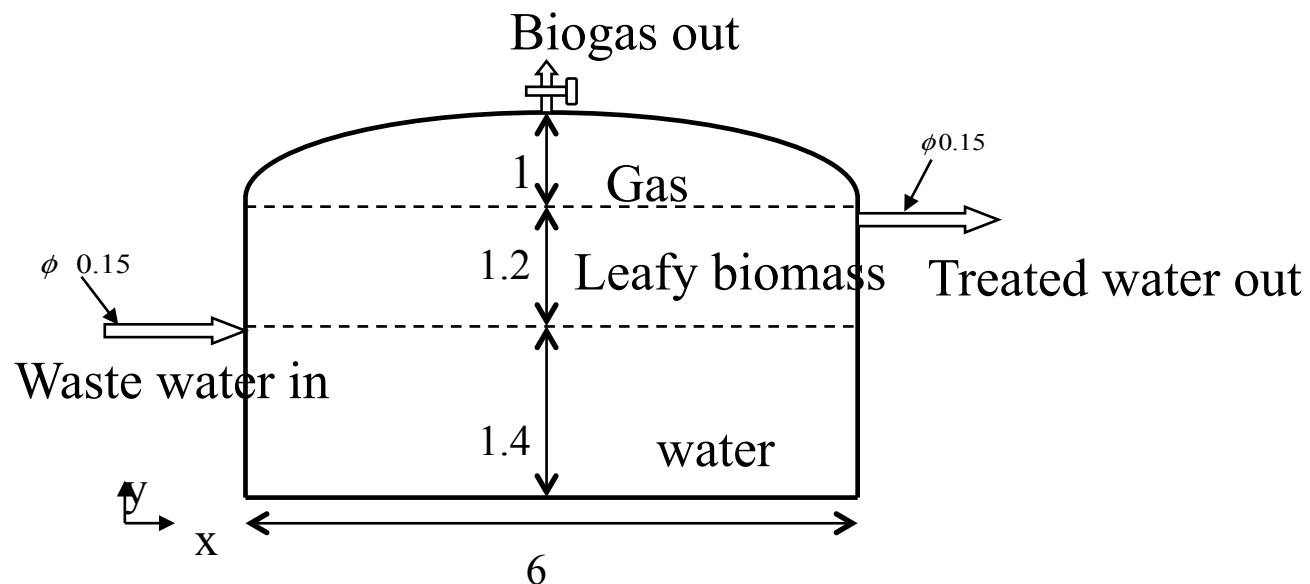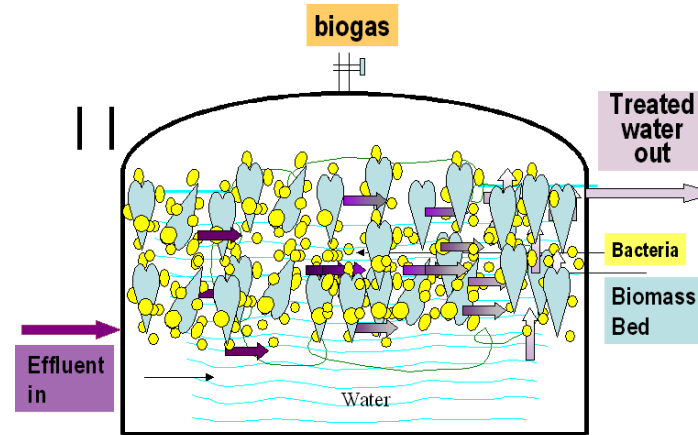
CFD modeling of bioreactors

➤ **Bioreactor performance: interactive relation between biosystem and physical environment**

- ❑ Biotic phase: complex machinary inside cell and its regulation by external environment

- ❑ Abiotic phase: multiphase system with complex interactions of mass, momentum and energy leading to environmental gradients in space and time
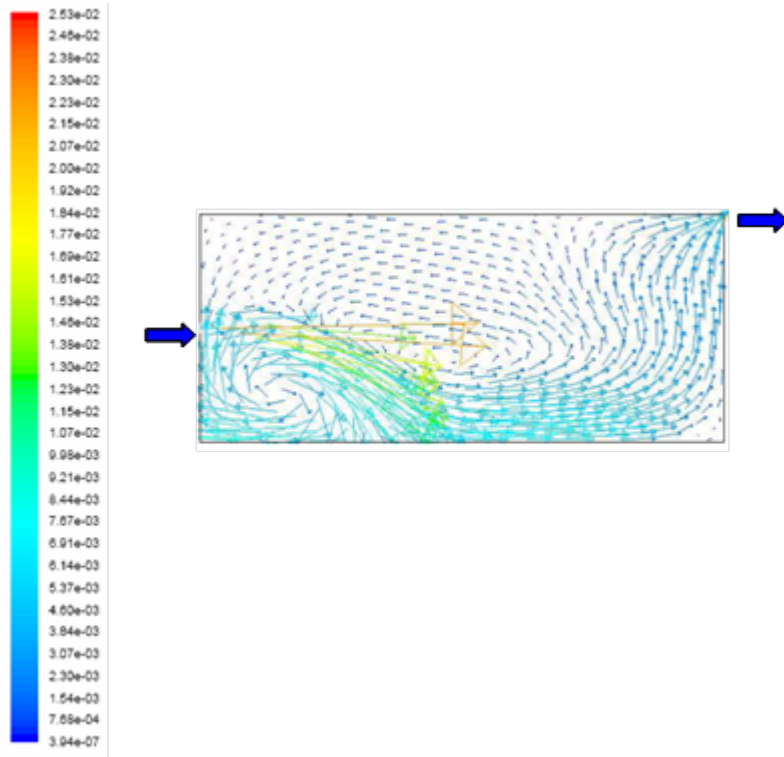
Anaerobic digestion

HYDROLYSIS and ACIDOGENESIS

ACETOGENESIS

METHANOGENESIS

Complex polymers

↓ *Fermentative B.*

Monomers

20

76 ↓ *Acidogenic B.*

4

Volatils fatty acids (VFA), alcohols, ...

Acetogenic B.

52   24

Acetate   → $CO_2 + H_2$

Homoacetogenic B.
Hydrogenophilic B.

72 ↓ *Acetoclastic B.*
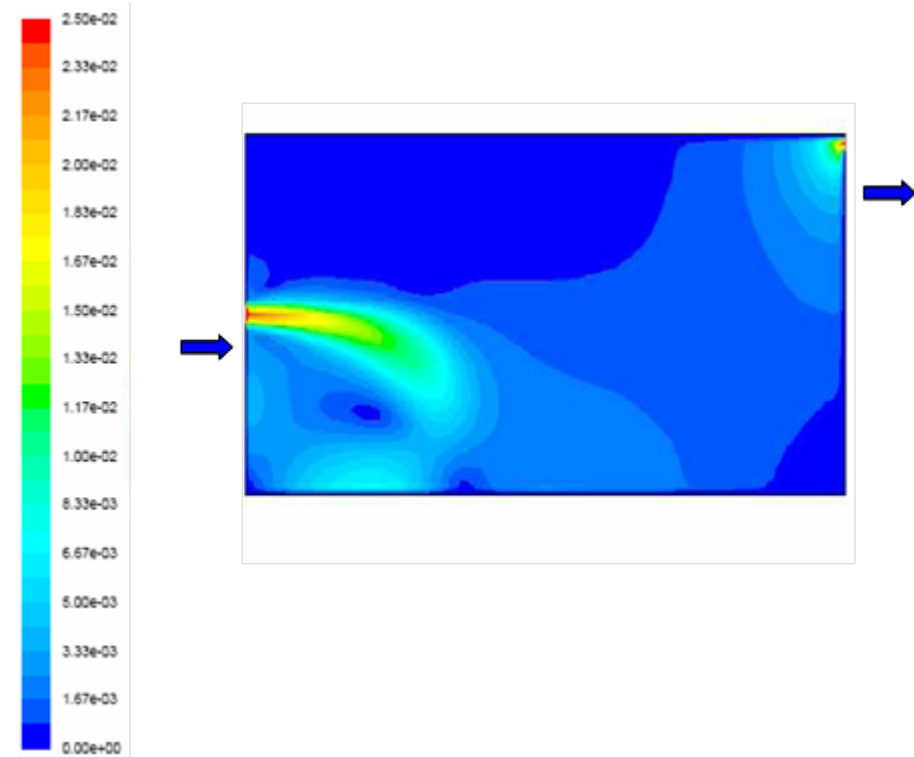
28

$CH_4 + CO_2$

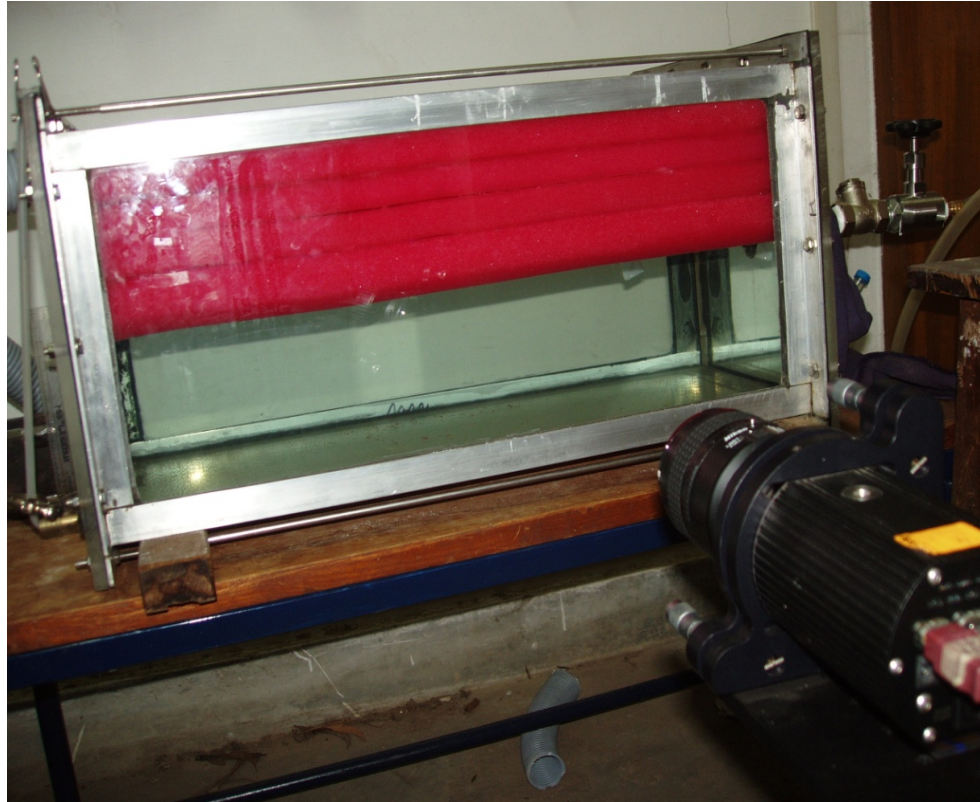$CH_4 + H_2O$

CFD modeling of anaerobic bioreactor

Results & Discussion
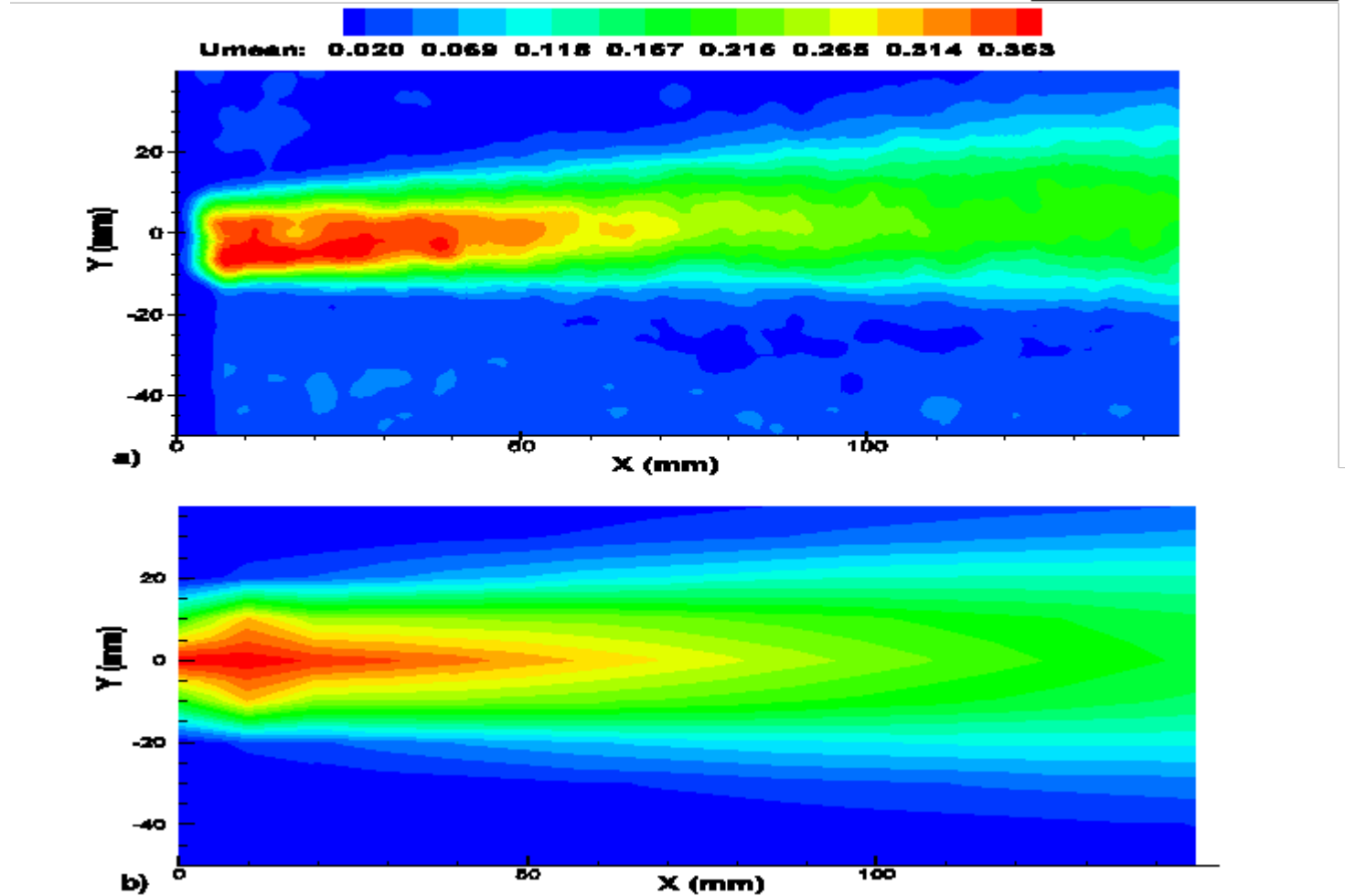

Vector plot for liquid velocity (m/s)
(with Packed bed)

Contour plot for liquid velocity (m/s)
(with Packed bed)

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PIV – experiments

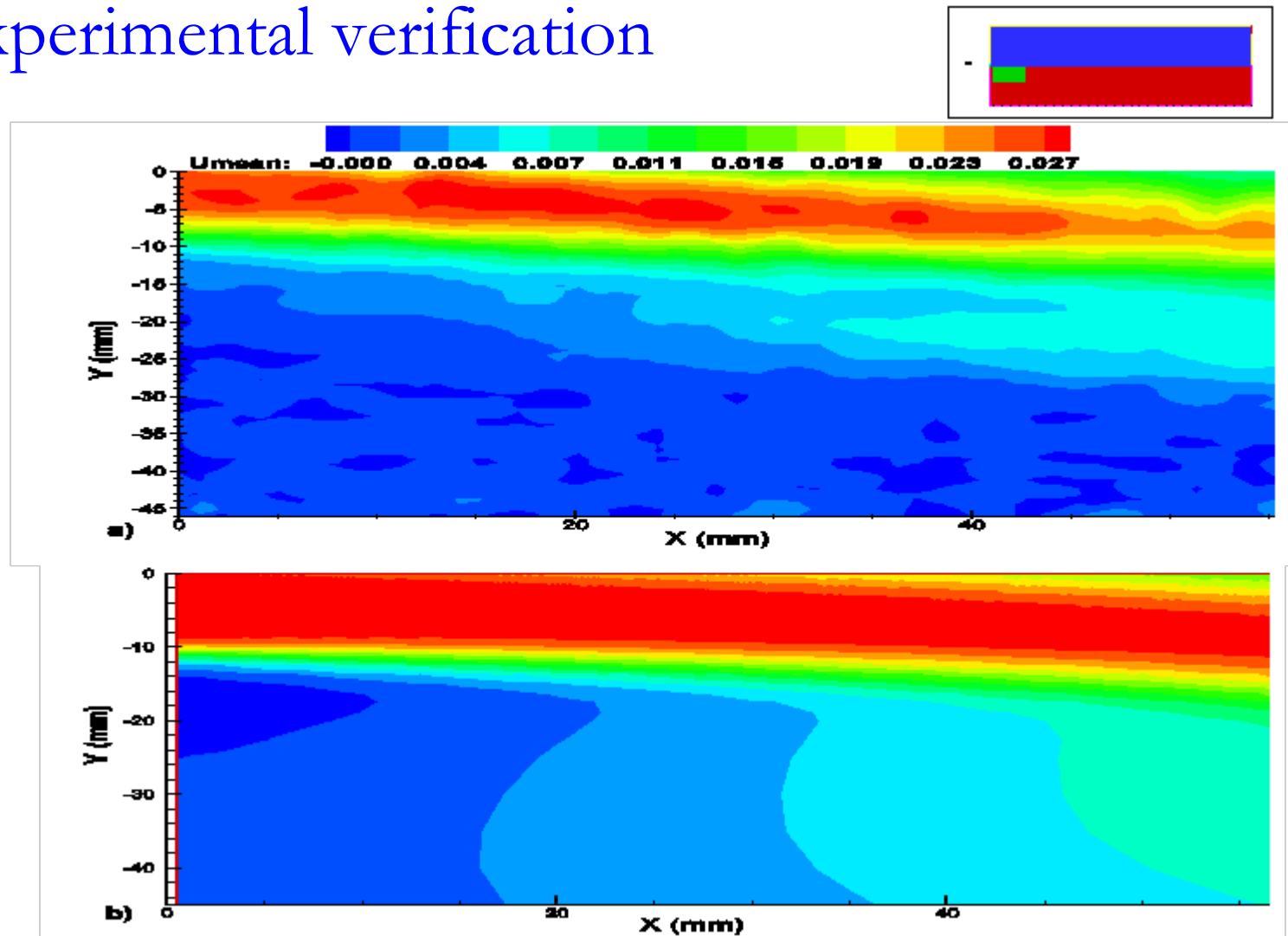# Experimental verification

Contours of X-direction mean velocity (inlet NRe=7660) (a)experimental and (b) Simulation results without packed bed

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Experimental verification
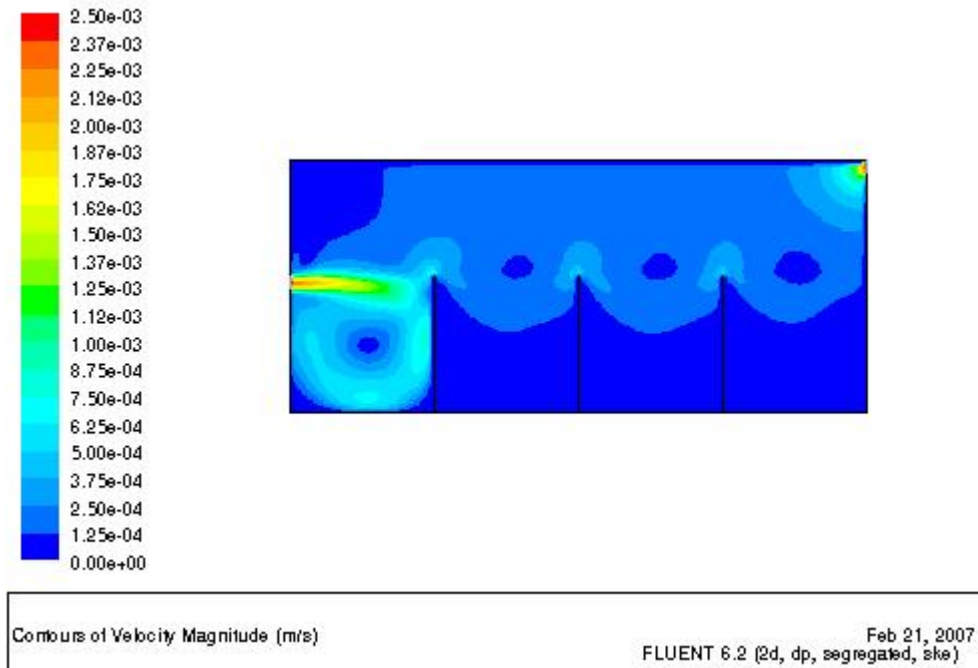

Contours of X-direction mean velocity (inlet NRe=500) (a)experimental and (b) Simulation results with packed bed

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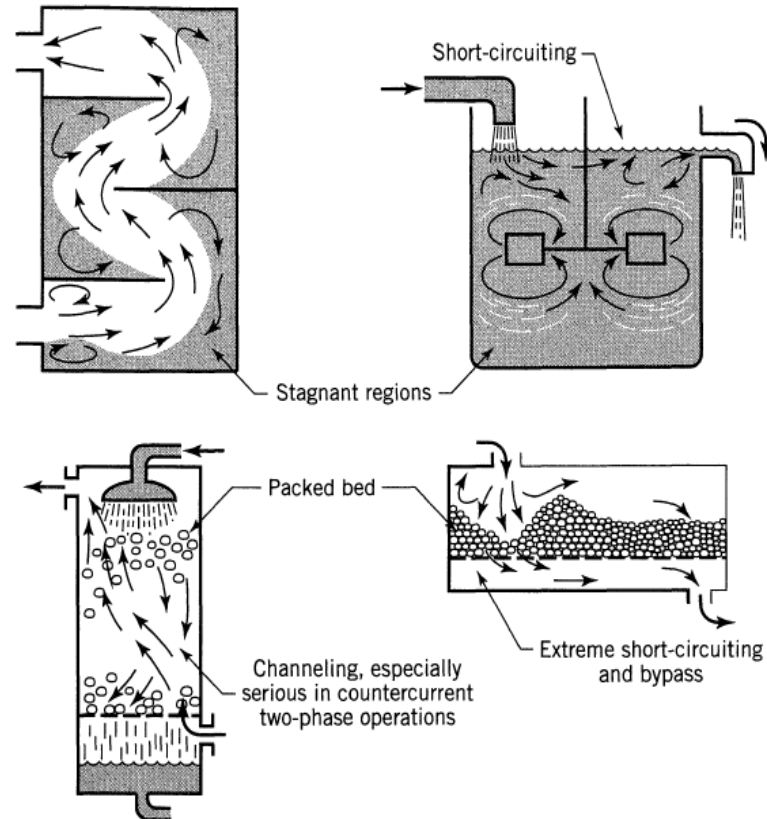# Improving the performance

Contours of Velocity Magnitude (m/s)   Feb 21, 2007
                                          FLUENT 6.2 (2d, dp, segregated, ske)
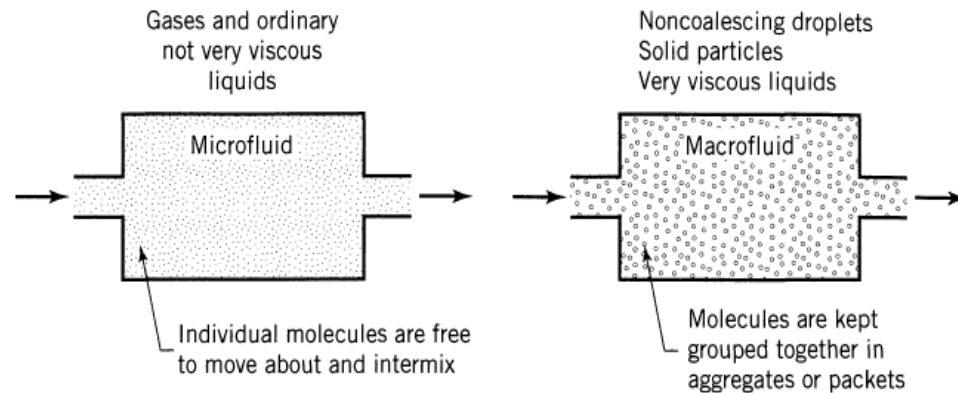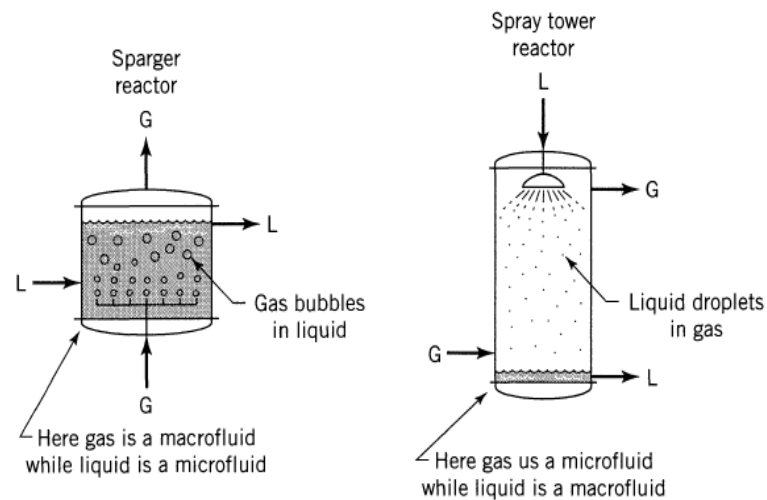
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Non-ideal flow, mixing and reactions

Figure 11.1 Nonideal flow patterns which may exist in process equipment.

Non-ideal flow, mixing and reactions

Gases and ordinary
not very viscous
liquids

Microfluid

Individual molecules are free
to move about and intermix

Noncoalescing droplets
Solid particles
Very viscous liquids

Macrofluid

Molecules are kept
grouped together in
aggregates or packets

Figure 11.2 Two extremes of aggregation of fluid.

Sparger
reactor

G

L

L

Gas bubbles
in liquid

G

Here gas is a macrofluid
while liquid is a microfluid

Spray tower
reactor

L

G

Liquid droplets
in gas

G
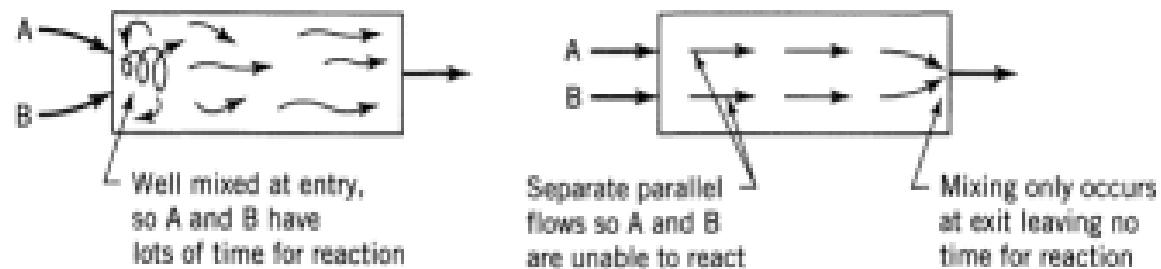
L

Here gas us a microfluid
while liquid is a macrofluid

Figure 11.3 Examples of macro- and microfluid behavior.

Non-ideal flow, mixing and reactions
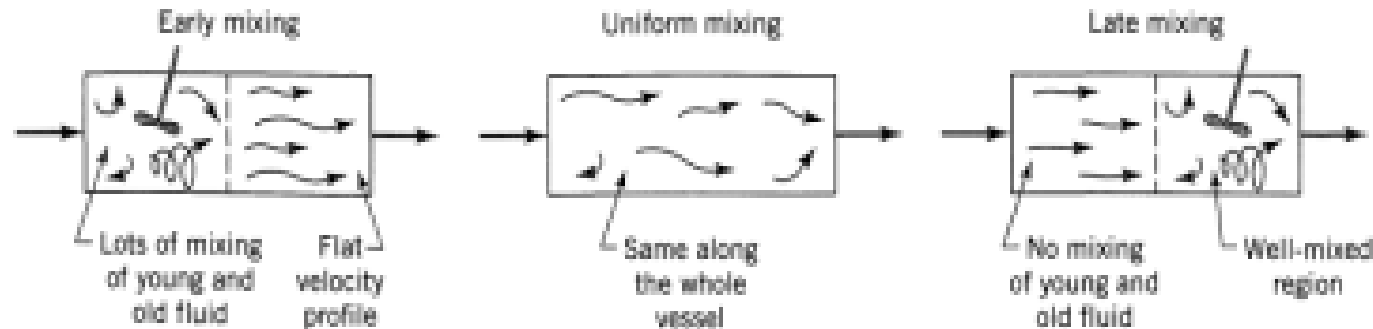
Figure 11.4 Examples of early and of late mixing of fluid.

Figure 11.5 Early or late mixing affects reactor behavior.

Residence time distributions

➤ Exit age distribution E(t)dt

❑ Fraction of material in exit stream which has age between t and t+dt

➤ Cumulative residence time distribution, F(t)

❑ Fraction of material in exit stream with age less than t

➤ Internal age distribution, I(t)dt

❑ Fraction of material within vessel which has age between t and t+dt

$$F(t) = \int_0^t E(t')dt' \ or \ \frac{dF(t)}{dt} = E(t), \qquad 1 - F(t) = \frac{V}{F'}I(t)$$

Means and moments of distribution

➢ Mean residence time

$$\bar{t} = \int_0^\infty tE(t)dt \left/ \int_0^\infty E(t)dt' = \int_0^\infty tE(t)dt \right.$$

➢ Variance

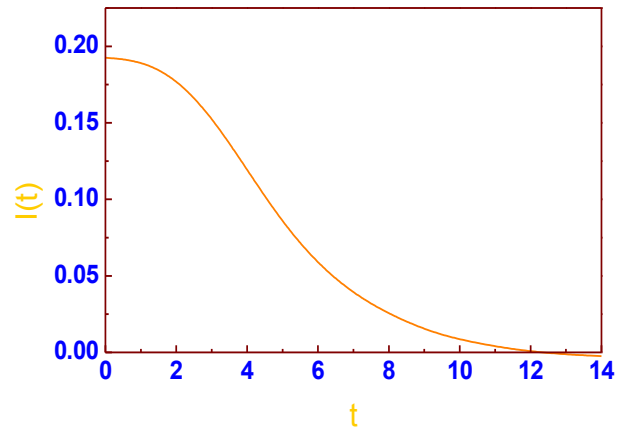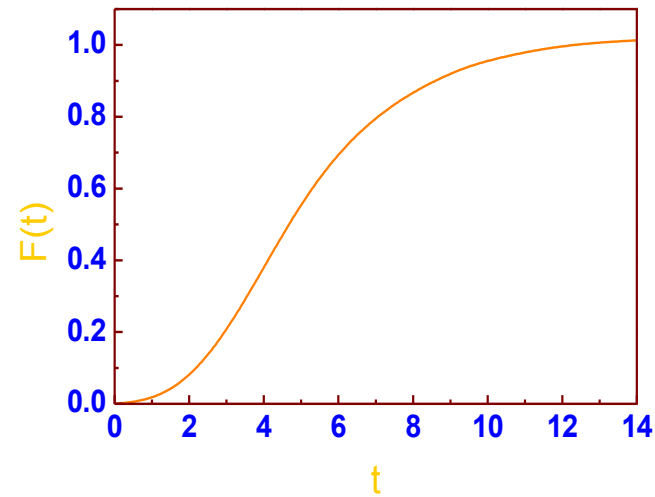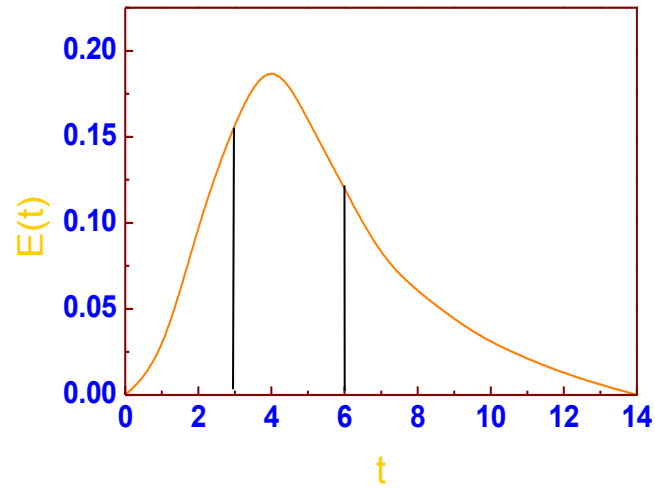$$\sigma^2 = \int_0^\infty \left(t - \bar{t}\right)^2 E(t)dt$$

➢ Skewness

$$s^3 = \int_0^\infty \left(t - \bar{t}\right)^2 E(t)dt \left/ \sigma^{3/2} \right.$$

Example
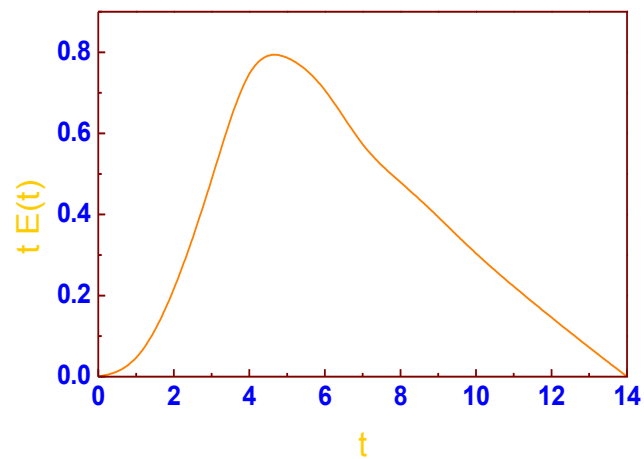
Experimental determination of RTD

➢ **Convolution integral**

$$C_e(t) = \int_0^t C_o(t - t')E(t')\,dt = \int_0^t C_o(t')E(t - t')\,dt$$

➢ **Pulse input**

$$E(t) = C_e(t) \Big/ \int_0^\infty C_e(t)\,dt$$

➢ **Step input**

$$F(t) = C_e(t) \big/ C_0$$

Determination of RTD from model

➢ CSTR

$$E(t) = \frac{1}{\tau} \exp\left(-t/\tau\right)$$
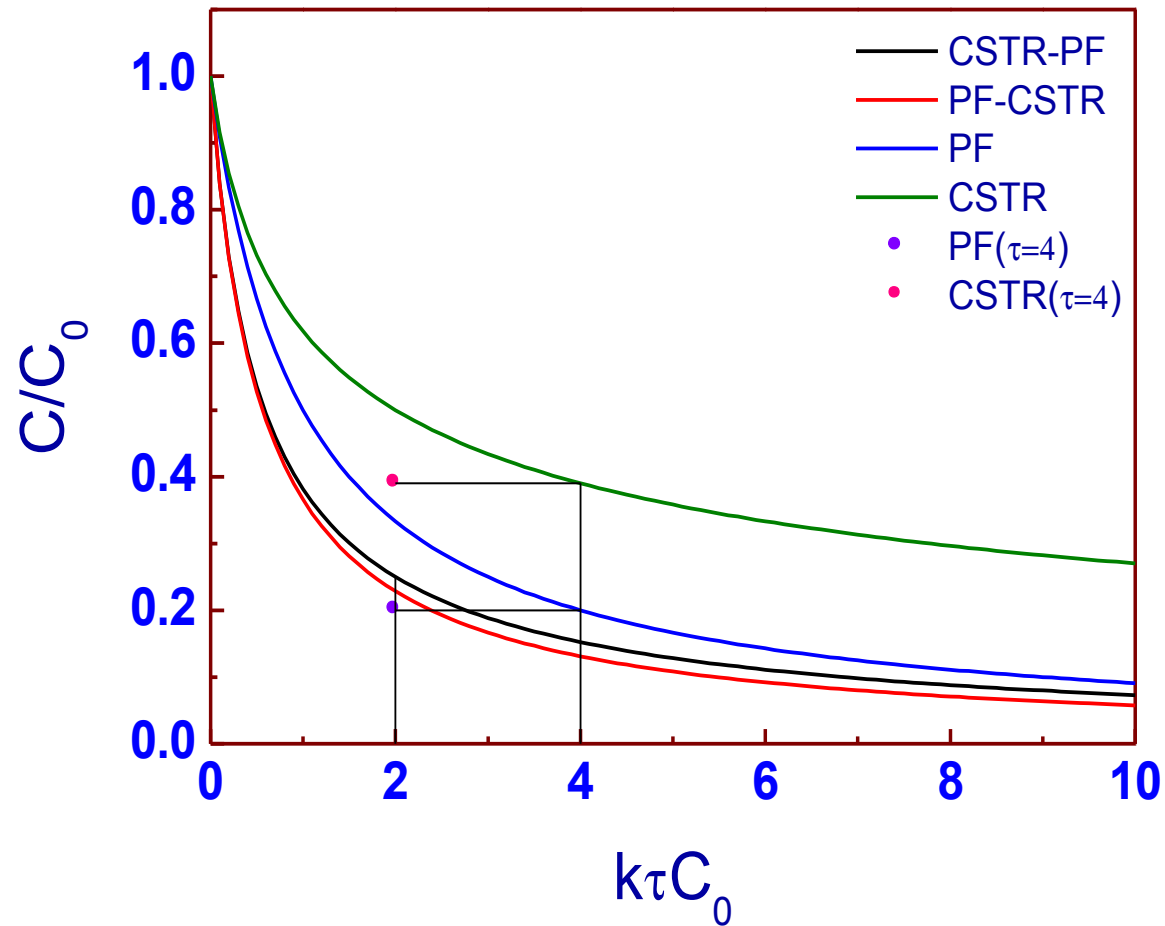
➢ PFR

$$E(t) = \delta(t - \tau), \ F(t) = H(t - \tau)$$

➢ PFR-CSTR or CSTR-PFR

$$E(t) = \begin{cases} 0 & t < \tau_p \\ \dfrac{1}{\tau_s} \exp\left(\dfrac{t - \tau_p}{\tau_s}\right) & t \geq \tau_p \end{cases}$$

RTD and reactions

- ➢ kinetics of the reaction
- ➢ the RTD of fluid in the reactor
- ➢ the earliness or lateness of fluid mixing in the reactor
- ➢ whether the fluid is a micro or macro fluid

Example – second order reaction

Macro- and Micromixing

- Macromixing – distribution of residence times in the reactor
- Micromixing – description of how molecules of different ages interaction with each other
  - Complete segregation – all molecules of same age group remain together until they exit the reactor
  - Complete micromixing – molecules of different age group are completely mixed
- the earliness or lateness of fluid mixing in the reactor
- whether the fluid is a micro or macro fluid

Zero parameter models

➢ **Complete segregation**
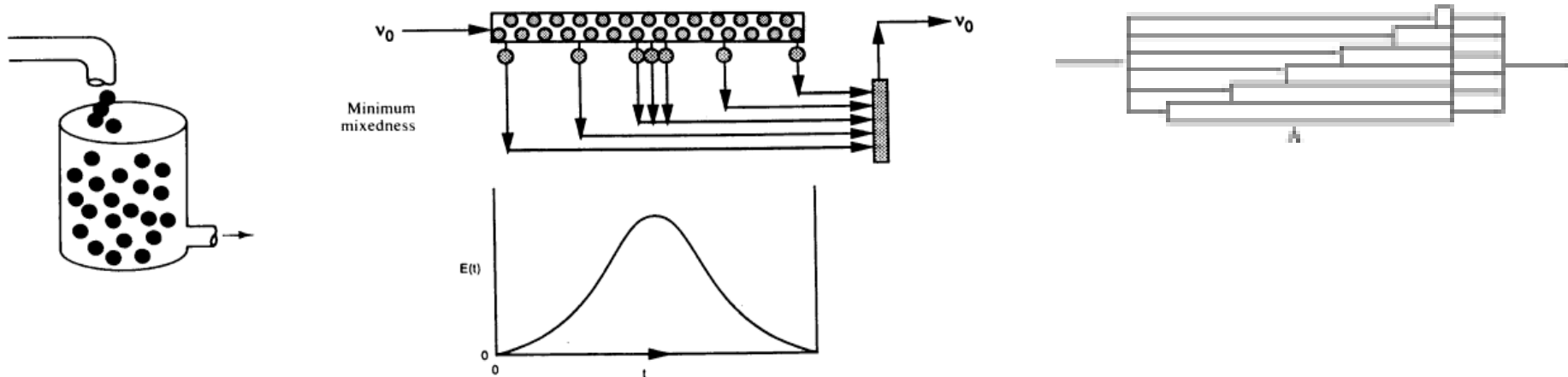
$$C_s = \int_0^\infty C(t)E(t)dt$$

Model

$$\frac{dC}{dt} = R(C) \quad C(0) = C_0 \qquad\qquad C_s = \int_0^\infty C(t)E(t)dt$$

$$\frac{dC_s}{dt} = C(t)E(t) \quad C_s(0) = 0$$

$$t = \frac{z}{z-1} \quad t(0,\infty) \equiv z(0,1) \qquad \frac{dC}{dt} = \frac{dC}{dz}\frac{dz}{dt} = (1-z)^2 \frac{dc}{dz}$$

$$\frac{dC}{dz} = \frac{R(C)}{(1-z)^2}$$
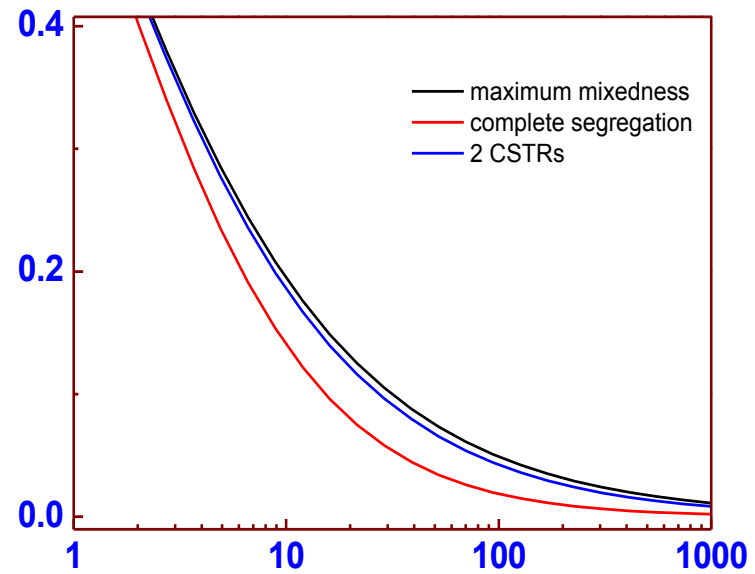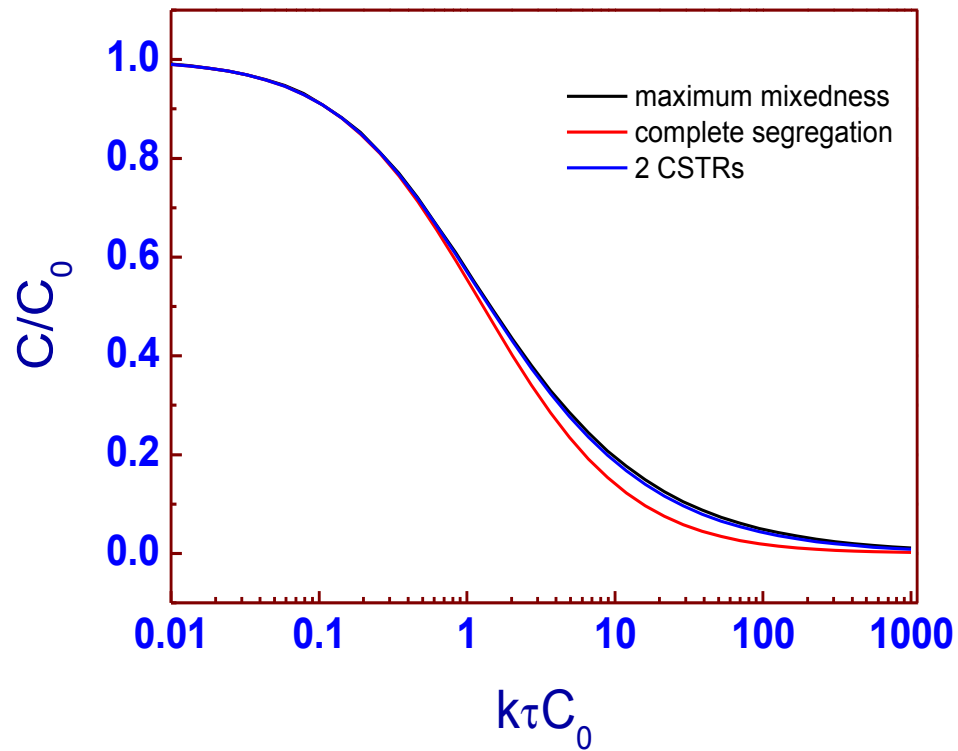
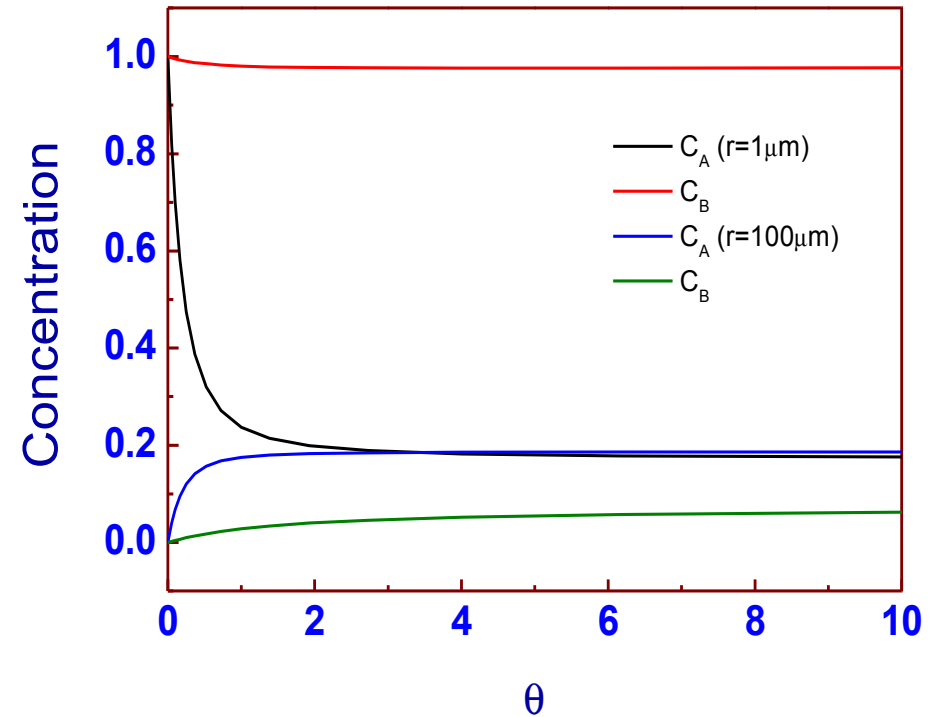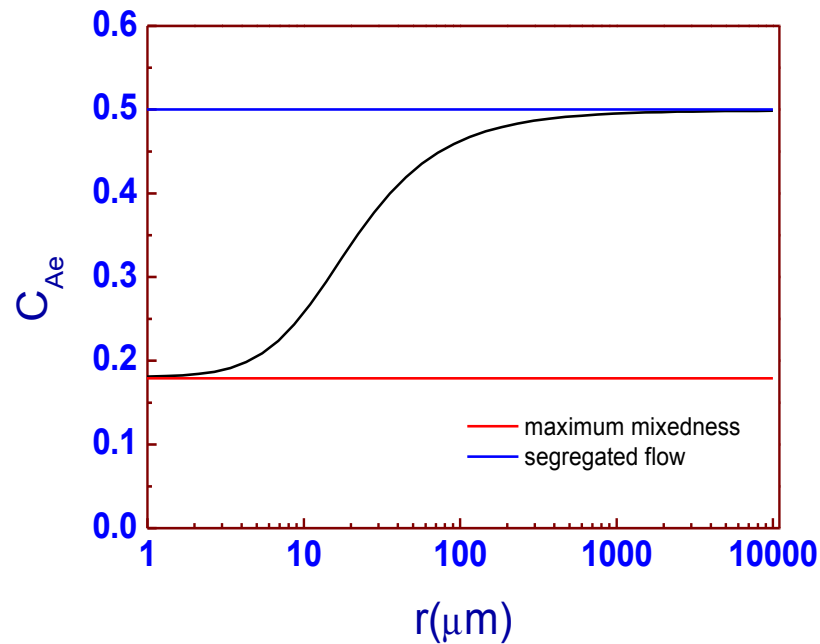$$\frac{dC_s}{dz} = \frac{E(z/1-z)}{(1-z)^2} C$$

Zero parameter models

➢ Maxiumum mixedness
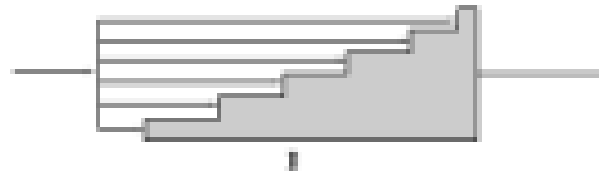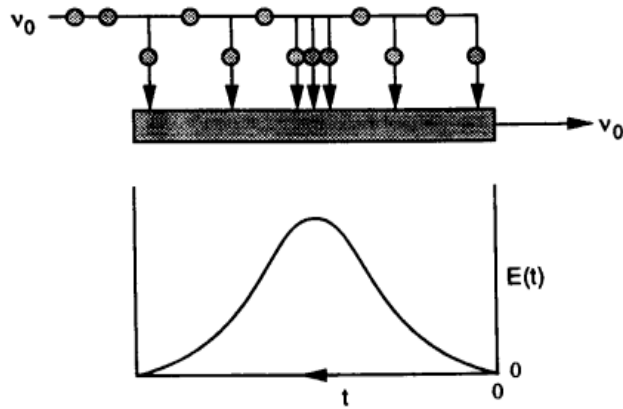
$$\frac{dC}{d\lambda} = -R(C) - (C_{10} - C)\frac{E(\lambda)}{1 - F(\lambda)} \qquad C(\lambda = 0) = C_{10}$$

Example – second order reaction

Example – mass transfer and reaction

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One parameter models

➢ Tanks – in - series
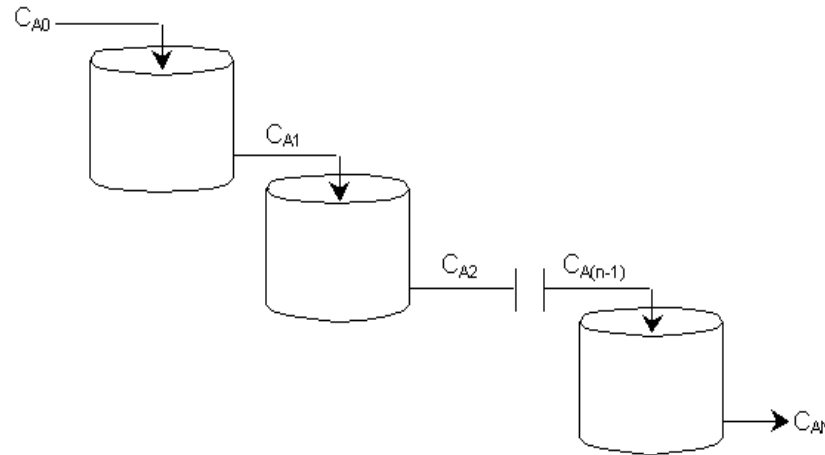
$$E(t) = \frac{N^N t^{n-1}}{(N-1)! \tau^N} \exp\left(\frac{nt}{\tau}\right) \qquad \sigma^2 = \frac{1}{N}$$
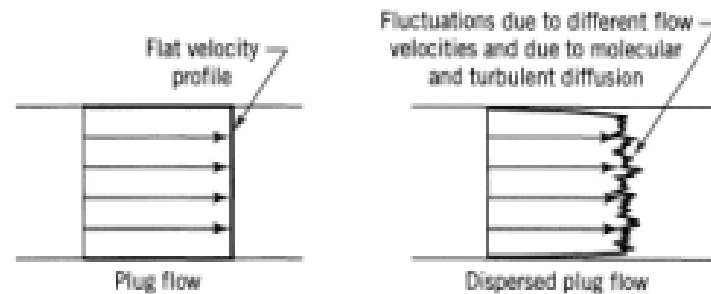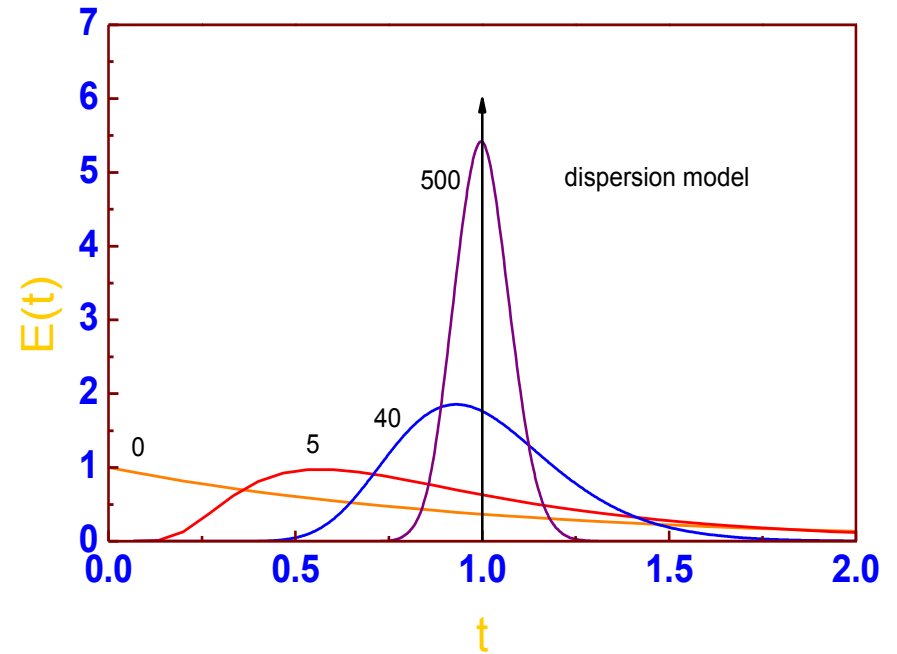
One parameter models
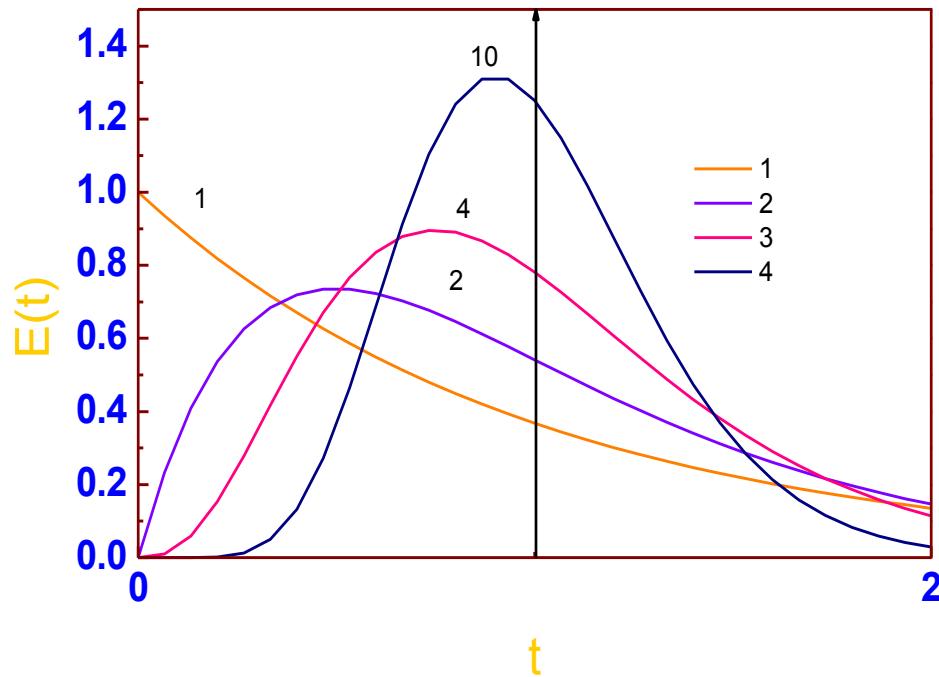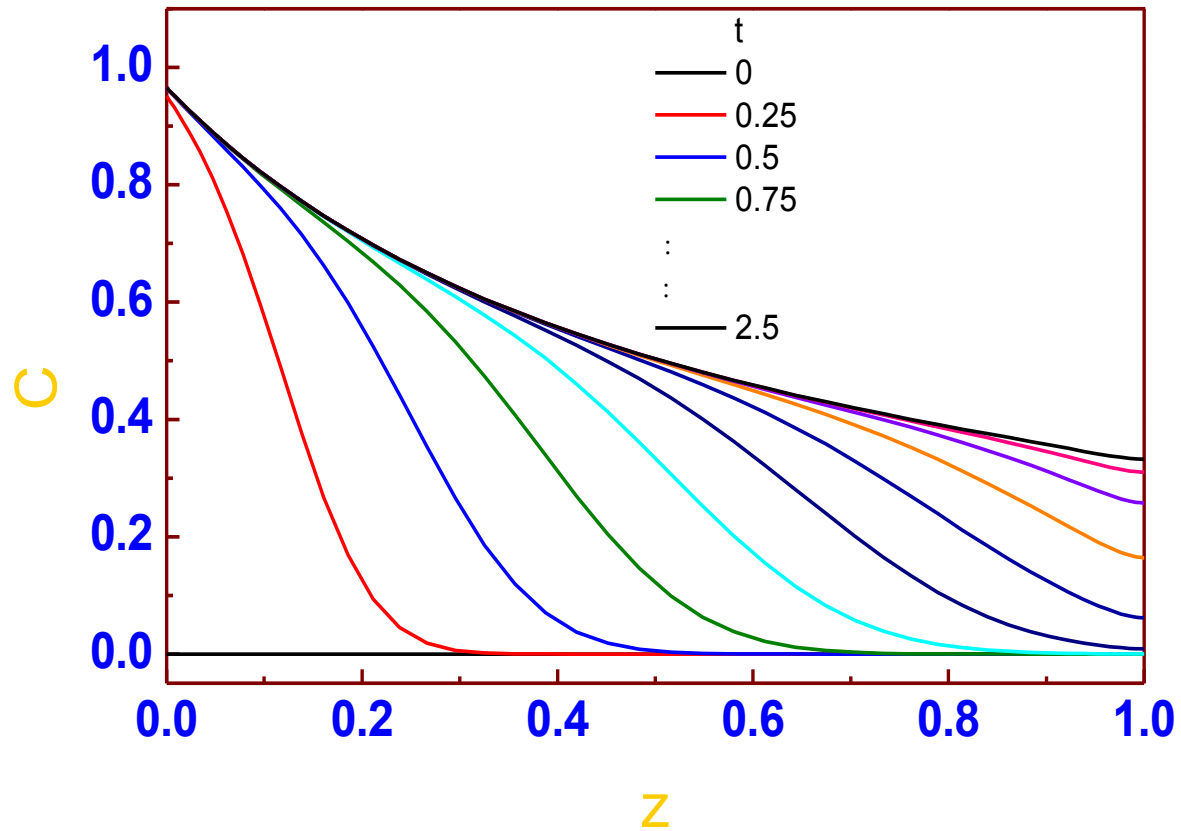
> ## Axial dispersion model

Figure 13.3 Representation of the dispersion (dispersed plug flow) model.

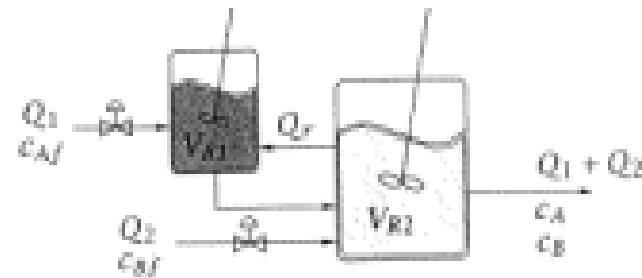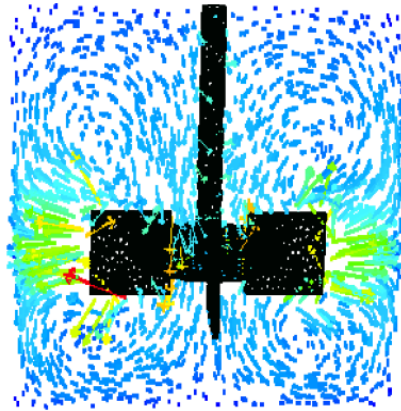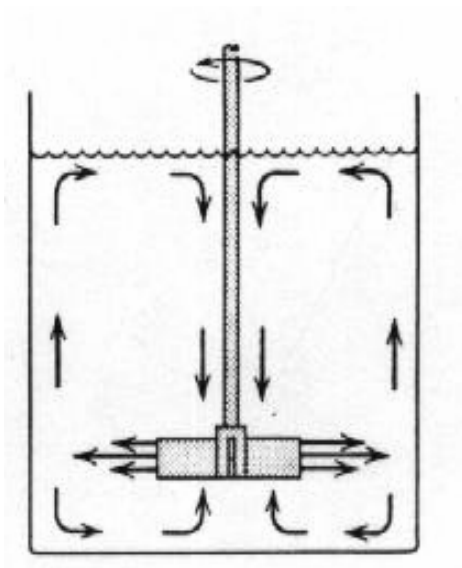$$\sigma^2 = \frac{1}{Pe}\left[1 - \frac{1}{Pe}\left(1 - e^{-Pe}\right)\right]$$
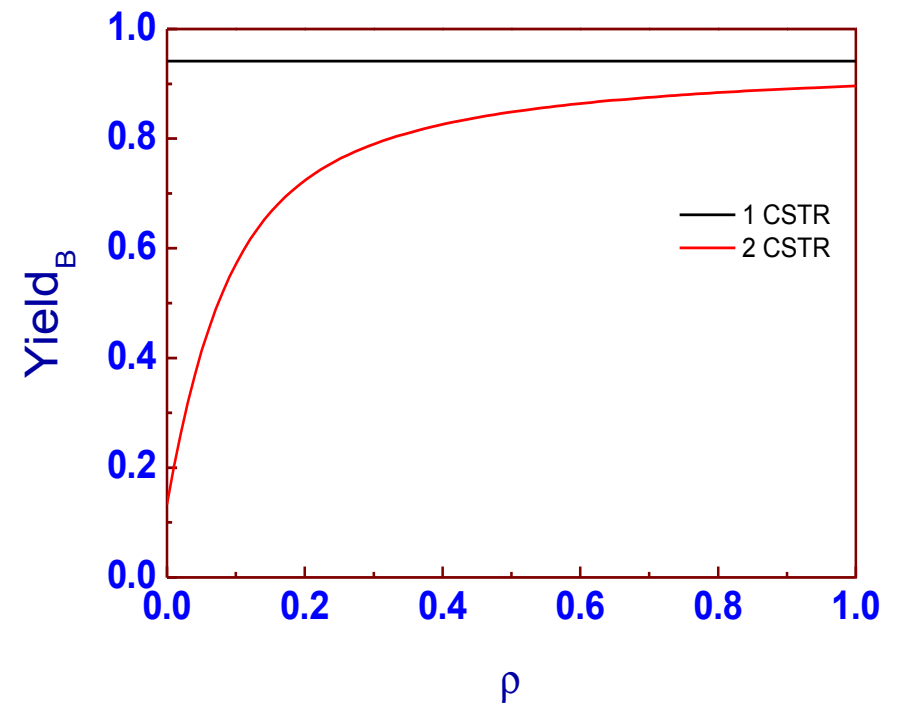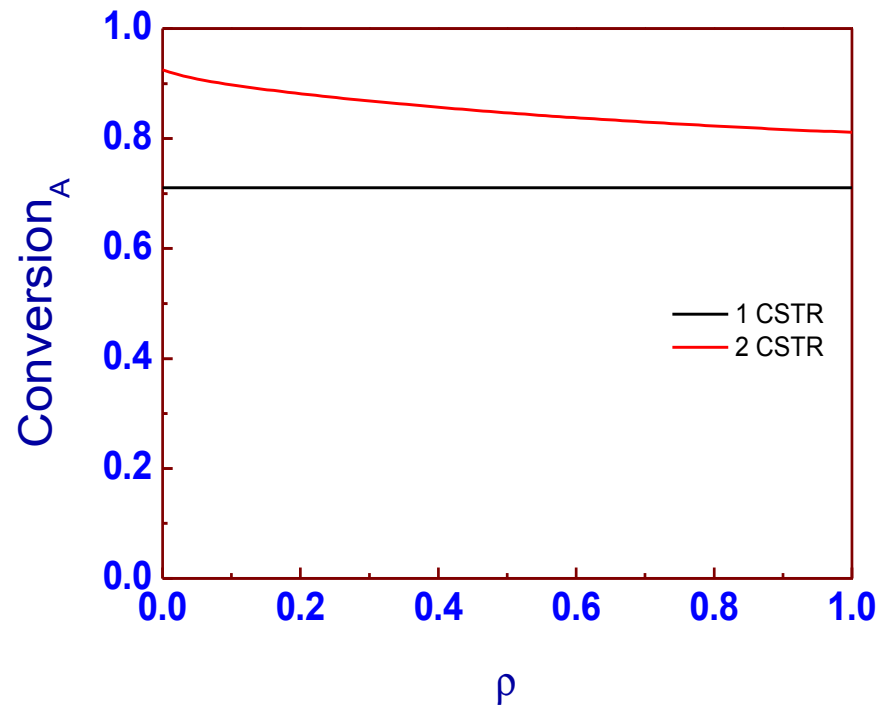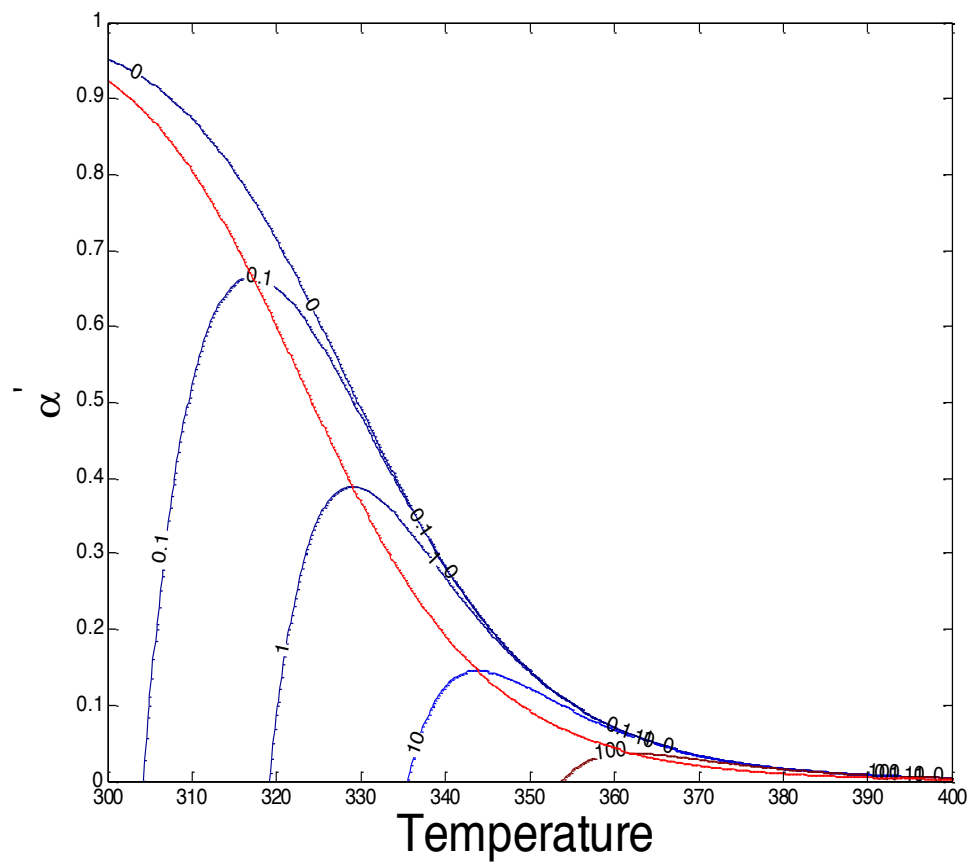
RTD

Transient in PFR

Compartment models

Example

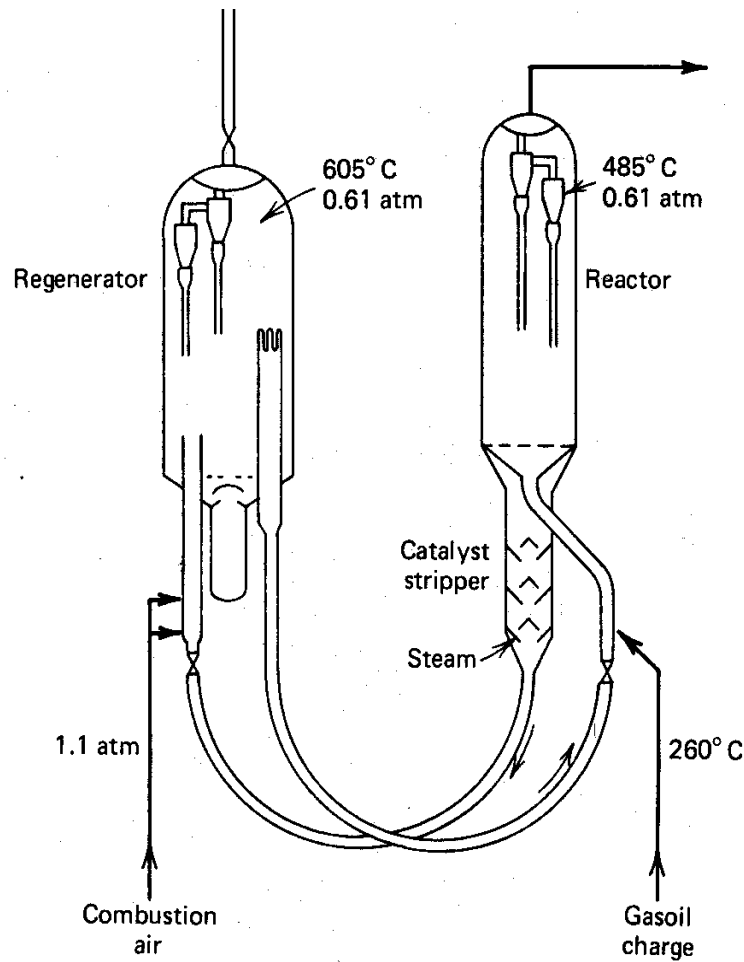# Rate contours –reversible reaction

Fludized bed catalytic convertors

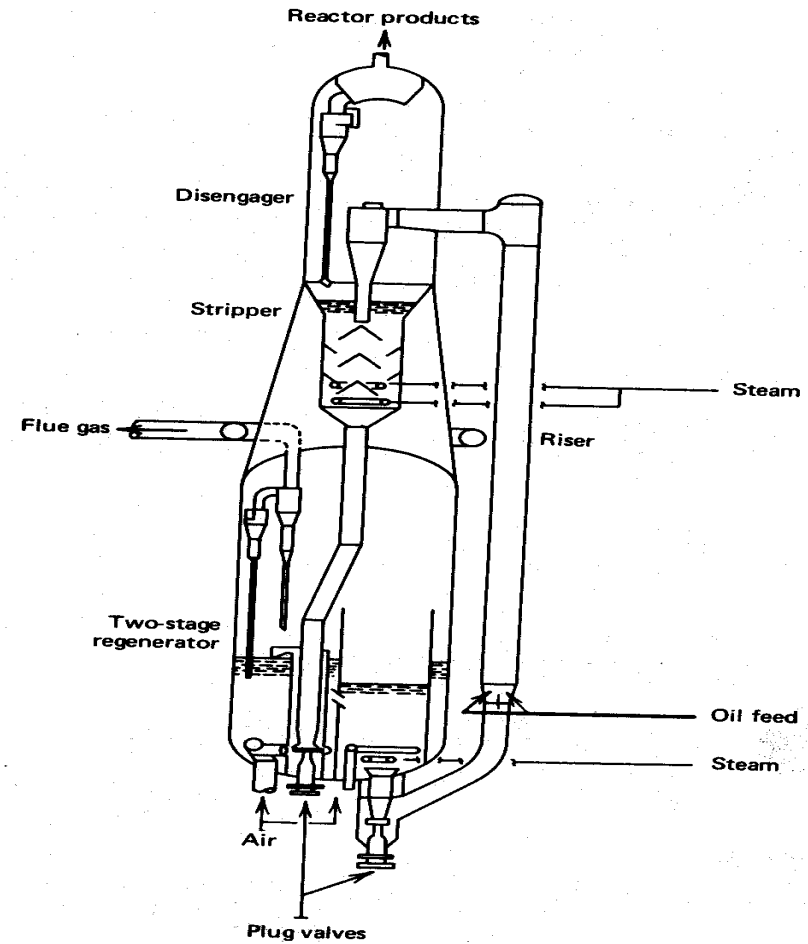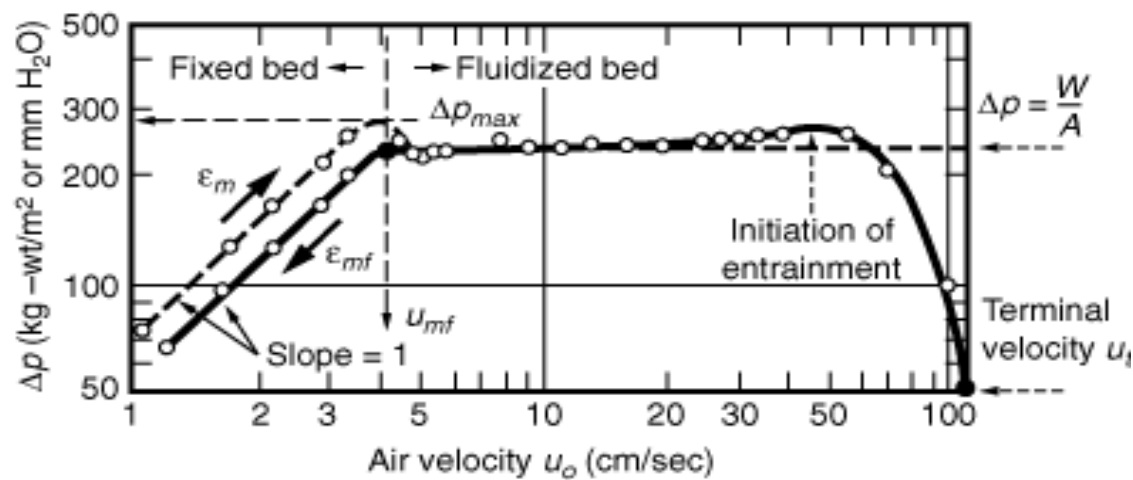Figure 13.2-1 Reactor-regeneration system for catalytic cracking of gasoil (after Zenz and Othmer [10]).
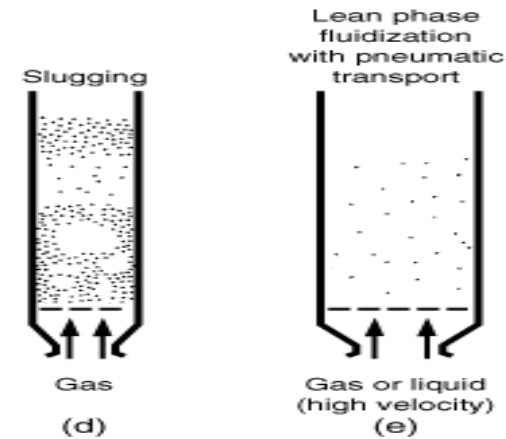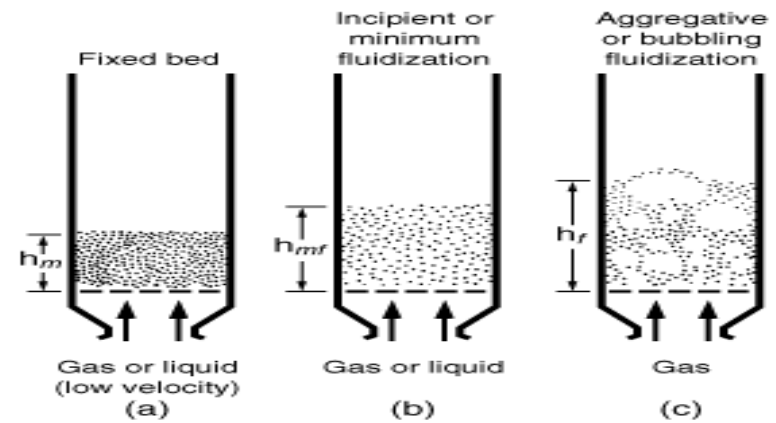

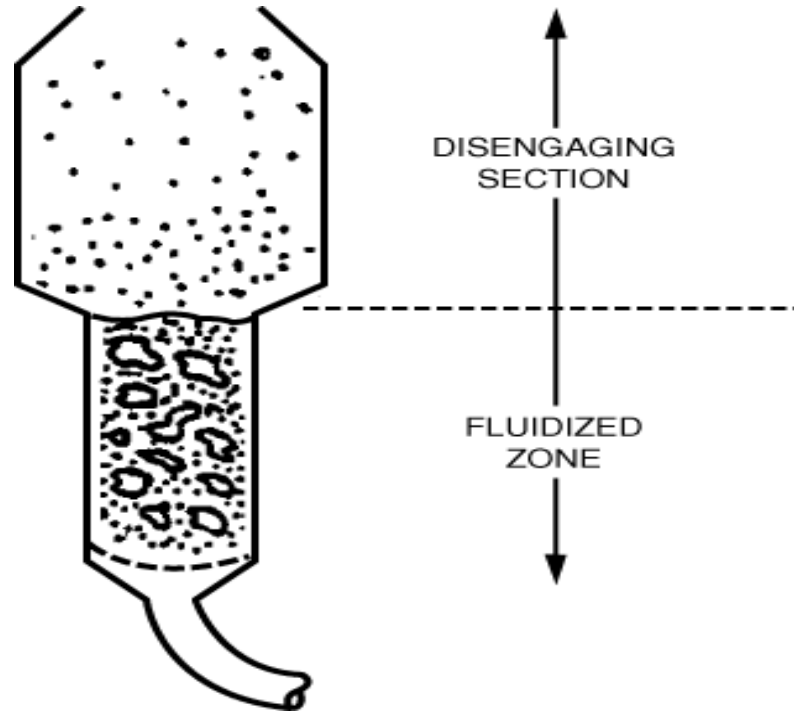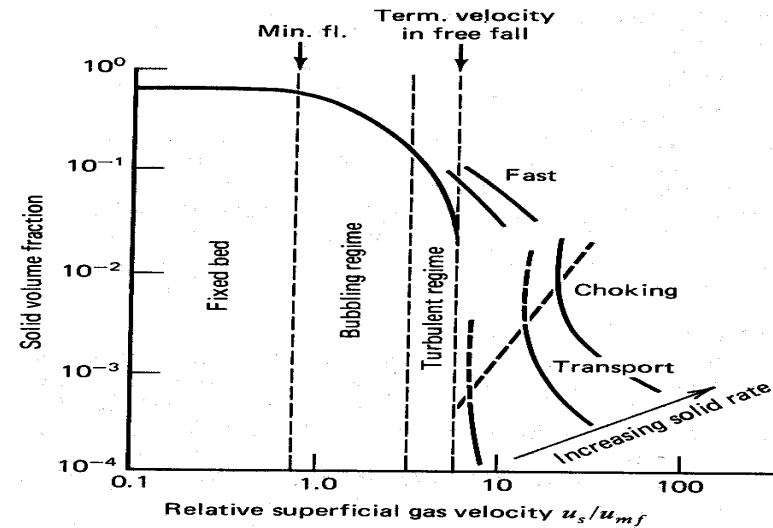Figure 13.2-2 Kellogg orthoflow model F convertor with riser cracking and two-stage regeneration (from Murphy and Soudek [30]).

Fluidised bed reactor

DISENGAGING SECTION

FLUIDIZED ZONE

Fixed bed

h_m

Gas or liquid (low velocity)

(a)

Incipient or minimum fluidization

h_{mf}

Gas or liquid

(b)

Aggregative or bubbling fluidization

h_f

Gas

(c)

Slugging

Gas

(d)

Lean phase fluidization with pneumatic transport

Gas or liquid (high velocity)

(e)

Fixed bed ← | → Fluidized bed

Δp_{max}

ε_m

ε_{mf}

Slope = 1

u_{mf}

Initiation of entrainment

$\Delta p = \dfrac{W}{A}$

Terminal velocity u_t

Air velocity u_o (cm/sec)

Δp (kg –wt/m² or mm H₂O)

Emulsion

Cloud

Bubble
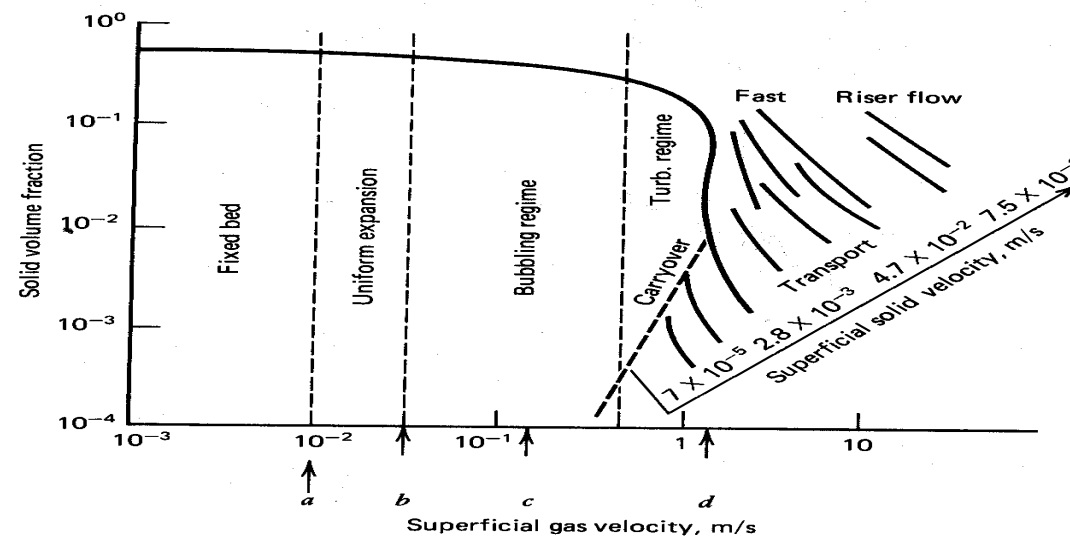
Wake

Solid volume fraction

Figure 13.3-4
Fluidization regimes with coarse particles. After Squires et al. (1985).

Figure 13.3-5
Fluidization regimes with fine particles. After Squires et al (1985). (*a*) Minimum buoyancy. (*b*) Minimum bubbling. (*c*) Terminal velocity. (*d*) Blowout velocity.

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