Making Friends with Chemical Reactors

by

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Narrated by: M.P. Dudukovic
I ♥ you
Making friends with reactors and knowing their habits is important.
Cowboy
My First Assignment as a Process Engineer (1967)

EUROPEAN (GERMAN) PROCESS:

**Carbon + Sulfur**

$\text{C} + 2\text{S}$

→ Electric arc

**Carbon Disulfide**

$\text{CS}_2$

**Reactor:** Refractory lined kiln with graphite electrodes
Reactor Clearly Environmentally Unfriendly!

Glowing Red Hot Coal!!!

Poisonous Gases!!!

VOLCANIC ERUPTIONS ONCE A WEEK (on the average)!!!

THAR’ IT BLOWS!!!

Reactor Clearly Environmentally Unfriendly!
• Runaway caused by thermal instability and ‘hot spots’ in the reactor – not controllable
• Recommendation of young engineers to the boss: “Prevolatize the sulfur and suspend smaller coke particles in sulphur vapor – run the process in a fluidized bed”

• Boss’s Response
  “No way! You know nothing about fluidization technology! Go improve on the German kilns!”
• Conclusion
  The “improved design of the “German” kilns (positioning more bottom electrodes to expand the hot zone) led to “our” kilns erupting once every two to three weeks (a big improvement according to our boss)

MORALE
If pollution was part of the cost, risk would have been taken to go for new technology. Without it no new process.

EPILOGUE
Four years after our recommendation a Japanese company proved fluidized bed concept viable.
Rule 1 For Single Reactions

Given $A \rightarrow R$, with rate $= kC_A^n$

$C_{Ao} \rightarrow \text{volume } V \rightarrow C_A, X_A$

to minimize $V$ keep $C_A$ as high as possible
\[ \frac{dA}{dt} = -r_A = kC_A^2 \]

\[ C_{AD} = 1000 \quad \rightarrow \quad \text{Reactor} \quad \rightarrow \quad C_A = 1 \]

mixed flow
\[ H = 1000 \text{m} \]

plug flow
\[ H = 1 \text{m} \]

Empire State
Rule 2 For Reactions in Series

Given \[ A \rightarrow R \rightarrow S \rightarrow T \ldots \] to maximize any intermediate do not mix fluids of different compositions.
Fluid Catalytic Cracking

\[ C_{18} \rightarrow C_{12} \rightarrow C_{8} \rightarrow C_{4} \rightarrow C \ldots \text{all endothermic} \]

Mixed

Plug
No. of units: 0-20-400-1
Capacity: 2000-140000 bbl/day
Average: 38000 bbl/day = 6000 m³/day
Value: $1 000 000/yr for a 1% increase
To Color Cola Drinks

sugar syrup → dark brown (caramelized) → carbon heat

155°C heat
Rule 3  For Reactions in Parallel

\[ R \quad r_R = k_0 \quad \text{lowest order} \]
\[ A \xrightarrow{S} \quad r_S = k_1 C_A \quad \text{intermediate order} \]
\[ T \quad r_T = k_2 C_A^2 \quad \text{highest order} \]

To maximize \( R \) ... operate at lowest \( C_A \)

To maximize \( S \) ... ?

To maximize \( T \) ... operate at highest \( C_A \)
\[
\begin{align*}
R &: r_R = k_0 \\
S &: r_S = k_1 C_A \\
T &: r_T = k_2 C_A^2
\end{align*}
\]

\[
\begin{align*}
\text{how to maximize } \frac{r_S}{-r_A} \\
\text{To find what } C_A \text{ will maximize } \frac{r_S}{-r_A} \text{ take } \\
\frac{d}{dc_A} \left( \frac{r_S}{-r_A} \right) = 0 = \frac{d}{dc_A} \left( \frac{k_1 C_A}{k_0 + k_1 C_A + k_2 C_A^2} \right) \\
= \frac{k_1 (k_0 + k_1 C_A + k_2 C_A^2) - k_1 C_A (k_1 + 2k_2 C_A)}{(\ldots \ldots)^2} \\
\therefore C_{A, \text{opt}} = \sqrt{\frac{k_0}{k_2}} \quad \text{... this particular } C_A \text{ is best.}
\end{align*}
\]
Rule 4  Complex Reactions

These can be analyzed by their component simple reactions, for example

\[
\begin{align*}
A + B &\rightarrow R \\
R + B &\rightarrow S
\end{align*}
\]

\[
\begin{align*}
A &\rightarrow R \rightarrow S \\
B &\leftrightarrow R \\
S &\leftrightarrow R
\end{align*}
\]
Industrial Example - Auto Antifreeze

\[ \text{EtOOH} + \text{H}_2\text{O} \rightarrow \text{EtO}_x \]

\[ \text{CH}_2\text{-CH}_2\text{OH} + \text{CH}_2\text{-CH}_2\text{OH} \rightarrow \text{CH}_2\text{-CH}_2\text{OCH}_2\text{CH}_2\text{OH} \]

\[ \text{A} + \text{B} \rightarrow \text{R} \]

\[ \text{EtO}_x \rightarrow \text{H}_2\text{O} \]

\[ \text{EtO}_x \rightarrow \text{EtO}_x \]
CONVENTIONAL PROCESS:
1. Plug flow reactor
2. Large excess water in the feed
3. Optimal residence time
4. Downstream separation – large separation train

PROPOSED PROCESS:
1. Reactive Distillation

ADVANTAGE:
Remove wanted product in situ as it is formed;
Make excess water available in reaction zone
OPTIMAL DISTRIBUTED FEED REACTIVE DISTILLATION COLUMN FOR ETHYLENE GLYCOL SYNTHESIS
Given $A_{\text{cells}} \rightarrow R + C$... rate $= \frac{kCA_{e}}{C_{A} + C_{M}}$

which reactor could be optimum, and which can never be (optimum = minimize volume).

$X_{A} = 0.9$

$C_{A0} = D$
Fig. 2. Reactor superstructure with three CSTRs.
Constraints:

(i) Molar balances for feed stream splitters

\[ FD_m - \sum_{i \in I} FR_{i,m} = 0 \quad m \in M^{mf} \]

(ii) Molar balances for mixers prior to each reactor

\[ \sum_{k \in I} RR_{k,i} \cdot XOUT_{k,m} + MR_{i} \cdot XFIN_{m} \]
\[ + FR_{i,mf} - IN_{i} \cdot XIN_{i,m} = 0 \quad m \in M, \quad i \in ICSTR, \quad mf \in M^{mf} \]

\[ BP_{ip,sk-1} \cdot XINS_{ip,sk-1} + OUTS_{ip,sk-1} \cdot XOUTS_{ip,sk-1,m} \]
\[ + \sum_{i \in I} RRS_{i,ip,sk} \cdot XOUT_{i,m} + FRS_{ip,sk,mf} \]
\[ + MRS_{ip,sk} \cdot XFIN_{m} - BP_{ip,sk} \cdot XINS_{ip,sk,m} \]
\[ - INS_{ip,sk} \cdot XINS_{ip,sk,m} = 0 \quad ip \in IPFR, \quad sk \in SK \quad 1 < sk < N_{SK}, \quad m \in M \]

(iii) Molar balances for splitters of the PFR streams

\[ FR_{i,m} - \sum_{sk \in SK} FR_{S_{i,sk,m}} = 0 \quad i \in IPFR, \quad m \in M^{mf} \]

\[ RR_{i,ip} - \sum_{sk \in SK} RRS_{i,ip,sk} = 0 \quad i \in I, \quad ip \in IPFR \]

\[ MR_{i,m} - \sum_{sk \in SK} MRS_{i,sk} = 0 \quad i \in IPFR \]

\[ V_{i} - \sum_{sk \in SK} VS_{i,sk} = 0 \quad i \in IPFR \]

(iv) Molar balances for splitters in the outlet of each reactor

\[ \sum_{k \in I} RR_{i,k} \cdot XOUT_{i,m} + RM_{i} \cdot XOUT_{i,m} \]
\[ - OUT_{i} \cdot XOUT_{i,m} = 0 \quad i \in I, \quad m \in M \]

\[ BP_{ip,sk} \cdot XINS_{ip,sk} + OUTS_{ip,sk} \cdot XOUTS_{ip,sk,m} \]
\[ - OUT_{ip} \cdot XOUT_{ip,m} = 0 \quad ip \in IPFR, \quad sk \in SK \quad sk = N_{SK}, \quad m \in M \]
(v) Molar balances for final mixer and recycle splitters

\[ FIN \cdot XFIN_m + TR \cdot XFIN_m - \sum_{i \in I} RM_i \cdot XOUT_{i,m} = 0 \quad m \in M \]

\[ TR - \sum_{i \in I} MR_i = 0 \]

(vi) Molar balances around each reactor

\[ IN_i \cdot XIN_{i,m} - OUT_i \cdot XOUT_{i,m} - V_i \sum_{rp} v_{rp,m} R_{rp,i} = 0 \quad i \in I^{CSTR}, \ m \in M \]

\[ INS_{i,sk} \cdot XINS_{i,sk,m} - OUTS_i \cdot OUTS_{i,sk,m} - VS_{i,sk} \sum_{rp} v_{rp,m} RS_{rp,i,sk} = 0 \quad i \in I^{PFR}, \ m \in M. \]

The reaction rates \( R_{rp,i} \) and \( RS_{rp,sk,i} \) can be expressed as a general function \( f_p \) of the outlet stream concentrations times the reaction constant \( k \) as follows:

\[ R_{rp,i} = k_{rp} \cdot f_p(CN_{i,m}) = 0 \quad \text{for } rp \in RP, \ i \in I^{CSTR}, \ m \in M^{rp} \]

\[ RS_{rp,sk,i} = k_{rp} \cdot f_p(CNS_{i,sk,m}) = 0 \quad \text{for } rp \in RP, \ i \in I^{PFR}, \ sk \in SK, \ m \in M^{rp} \]

where the outlet concentrations are given in terms of molar fractions as

\[ CN_{i,m} \left( \sum_{m \in M} XOUT_{i,m} \cdot MV_m \right) - XOUT_{i,m} = 0 \]

\[ i \in I, \ m \in M \]

\[ CNS_{i,sk,m} \left( \sum_{m \in M} OUTS_{i,sk,m} \cdot MV_m \right) - OUTS_{i,sk,m} = 0 \quad i \in I^{PFR}, \ m \in M, \ sk \in SK \]

(vii) Summation of mole fractions

\[ \sum_{m \in M} XIN_{i,m} - 1 = 0 \quad i \in I \]

\[ \sum_{m \in M} XOUT_{i,m} - 1 = 0 \quad i \in I \]

\[ \sum_{m \in M} XINS_{i,sk,m} - 1 = 0 \quad i \in I^{PFR}, \ sk \in SK \]

\[ \sum_{m \in M} OUTS_{i,sk,m} - 1 = 0 \quad i \in I^{PFR}, \ sk \in SK \]

\[ \sum_{m \in M} XFIN_m - 1 = 0 \]
(viii) **Logical constraints**

Logical constraints that force the continuous variables associated with a nonactive unit to take the value of zero are

\[ IN_i - U \cdot Z_i \leq 0 \quad i \in I \]
\[ V_i - U \cdot Z_i \leq 0 \quad i \in I \]
\[ INS_{i, sk} - U \cdot ZS_{i, sk} \leq 0 \quad i \in IPFR, \quad sk \in SK \]
\[ VS_{i, sk} - U \cdot ZS_{i, sk} \leq 0 \quad i \in IPFR, \quad sk \in SK. \]

The parameter \( U \) is a large number which provides a reasonable upper bound for the variable if the unit is activated (i.e. \( Z_i \) or \( ZS_{i, sk} \) take the value 1). If, however, the unit is not selected (i.e. \( Z_i \) or \( ZS_{i, sk} \) take the value 0) the above inequalities force the positive continuous variables to zero values.

Another set of logical constraints describes logical sequences of units in the superstructure. These constraints are used in order to exclude a unit: from the solution (i.e. force its corresponding integer to take zero value) if either its preceding or its reference unit is not selected. The following constraints of this type were introduced:

\[ ZS_{i, sk} - Z_i \leq 0 \quad i \in IPFR, \quad sk \in SK \]
\[ ZS_{i, sk} - ZS_{i, sk-1} \leq 0 \quad i \in IPFR, \quad sk \in SK. \]

The mathematical formulation can, in general, handle all the proposed bypasses of the superstructure. In the considered examples the existence of a bypass around a SCSTR unit is associated with the existence of the particular unit according to the following logical constraints:

\[ BP_{i, sk} - U \cdot (1 - ZS_{i, sk}) \leq 0 \quad i \in IPFR, \quad sk \in SK. \]

Finally, since the reactor network should always be active:

\[ \sum_{i \in I} Z_i \geq 1. \]

(ix) **Nonnegativity and integrality constraints**

\[ FD_m, FR_{i, m}, MR_i, IN_i, OUT_i \geq 0 \]
\[ RM_i, FR_{i, sk, m}, MR_{i, sk}, INS_{i, sk} \geq 0 \]
\[ OUTS_{i, sk}, RSS_{i, k, sk}, BP_{i, sk}, XFIN_m \geq 0 \]
\[ XIN_{m, i}, XOUT_{i, sk, m}, XINS_{i, sk, m}, XOUTS_{m, i} \geq 0 \]
\[ V_i, VS_{i, sk}, R_{r, p, i, sk}, RS_{r, p, i, sk}, CN_{i, m}, CNS_{i, sk, m} \geq 0 \]
\[ Z_{i, sk} \in \{0, 1\}. \]

**Mathematical formulation**

\[ \text{MIN or MAX } \Psi(XIN_{m, i}, XFIN_m, V_i) \quad \forall i \in I, \quad m \in M \]

Subject to

\[ FD_m - \sum_{i \in I} FR_{i, m} = 0 \quad m \in M^m \]
\[
\sum_{k \in l} RR_{k,i} \cdot XOUT_{k,m} + MR_i \cdot XFIN_m + FR_{i,m}f
\]
\[
- IN_i \cdot XIN_{i,m} = 0 \\
m \in M, \ i \in I^{CSTR}, \ m \in M^{mf}
\]
\[
BP_{ip,sk} \cdot XINS_{ip,sk} - 1
\]
\[
+ OUT_{ip,sk} \cdot XOUT_{ip,sk} - 1, m
\]
\[
+ \sum_{i \in l} RRS_{ip,sk} \cdot XOUT_{i,m} + FR_{ip,sk, mf}
\]
\[
+ MRS_{ip,sk} \cdot XFIN_m - BP_{ip,sk} \cdot XINS_{ip,sk, m}
\]
\[
- INS_{ip,sk} \cdot XINS_{ip,sk, m} = 0 \\
i \in I^{PFR}, \ sk \in SK, \ 1 < sk < N_{SK}, \ m \in M
\]
\[
IN_{ip} \cdot XIN_{ip, m} + \sum_{i \in l} RRS_{ip,sk} \cdot XOUT_{i,m}
\]
\[
+ FR_{ip,sk, mf} + MRS_{ip,sk} \cdot XFIN_m
\]
\[
- BP_{ip,sk} \cdot XINS_{ip,sk, m} + 1
\]
\[
- INS_{ip,sk} \cdot XINS_{ip,sk, m} = 0 \\
i \in I^{PFR}, \ sk \in SK, \ sk = 1, \ m \in M
\]
\[
FR_{i,m} - \sum_{sk \in SK} FRS_{i,sk, m} = 0 \ i \in I^{PFR}, \ m \in M^{mf}
\]
\[
RR_{i,ip} - \sum_{sk \in SK} RRS_{i,ip,sk} = 0 \ i \in I, \ ip \in I^{PFR}
\]
\[
MR_{i,m} - \sum_{sk \in SK} MRS_{i,sk} = 0 \ i \in I^{PFR}
\]
\[
V_i - \sum_{sk \in SK} VS_{i,sk} = 0 \ i \in I^{PFR}
\]
\[
\sum_{k \in l} RR_{i,k} \cdot XOUT_{i,m} + RM_i \cdot XOUT_{i,m}
\]
\[
- OUT_i \cdot XOUT_{i,m} = 0 \ i \in l, \ m \in M
\]
\[
BP_{ip,sk} \cdot XINS_{ip,sk} + OUT_{ip,sk} \cdot XOUT_{ip,sk, m}
\]
\[
- OUT_{ip} \cdot XOUT_{ip, m} = 0 \\
i \in I^{PFR}, \ sk \in SK, \ sk = N_{SK}, \ m \in M
\]
\[
FIN \cdot XFIN_m + TR \cdot XFIN_m
\]
\[
- \sum_{ip \in I^{PFR}} RM_i \cdot XOUT_{i,m} = 0 \ m \in M
\]
\[
TR - \sum_{i \in I} MR_i = 0
\]
\[
IN_i \cdot XIN_{i,m} - OUT_i \cdot XOUT_{i,m}
\]
\[
- V_i \cdot \sum_{rp \in RP} v_{rp,m} \cdot R_{rp,i} = 0 \ i \in I^{CSTR}, \ m \in M
\]
\[
INS_{i,sk} \cdot XINS_{i,sk, m} - OUT_{i} \cdot XOUT_{i,sk, m}
\]
\[
- VS_{i,sk} \cdot \sum_{rp \in RP} v_{rp,m} \cdot R_{rp,i,sk} = 0 \ i \in I^{PFR}, \ m \in M
\]
\[
R_{rp,i} - k_{rp} \cdot f_{rp}(CN_{i,m}) = 0 \\
rp \in RP, \ i \in I^{CSTR}, \ m \in M^{rp}
\]
\[
\begin{align*}
RS_{rp,i,sk} - k_{rp} \cdot f_{rp}(CNS_{i,sk,m}) &= 0 \\
   rp &\in RP, \quad i \in I^{PFR}, \quad sk \in SK, \quad m \in M^{rp} \\
CN_{i,m} \left( \sum_{m \in M} XOUT_{i,m} \cdot MV_{m} \right) - XOUT_{i,m} &= 0 \\
   i &\in I, \quad m \in M \\
CNS_{i,sk,m} \left( \sum_{m \in M} XOUT_{i,sk,m} \cdot MV_{m} \right) \\
XOUT_{i,sk,m} &= 0 \quad i \in I^{PFR}, \quad m \in M, \quad sk \in SK \\
   \sum_{m \in M} XIN_{i,m} - 1 &= 0 \quad i \in I \\
   \sum_{m \in M} XOUT_{i,m} - 1 &= 0 \quad i \in I \\
   \sum_{m \in M} XINS_{i,sk,m} - 1 &= 0 \quad i \in I^{PFR}, \quad sk \in SK \\
   \sum_{m \in M} XOUTS_{i,sk,m} - 1 &= 0 \quad i \in I^{PFR}, \quad sk \in SK \\
   \sum_{m \in M} XFIN_{m} - 1 &= 0 \\
   \sum_{i \in I} Z_{i} &\geq 1 \\
   IN_{i} - U \cdot Z_{i} &\leq 0 \quad i \in I \\
   V_{i} - U \cdot Z_{i} &\leq 0 \quad i \in I \\
   INS_{i,sk} - U \cdot ZS_{i,sk} &\leq 0 \quad i \in I^{PFR}, \quad sk \in SK \\
   VS_{i,sk} - U \cdot ZS_{i,sk} &\leq 0 \quad i \in I^{PFR}, \quad sk \in SK \\
   ZS_{i,sk} - Z_{i} &\leq 0 \quad i \in I^{PFR}, \quad sk \in SK \\
   ZS_{i,sk} - ZS_{i,sk-1} &\leq 0 \quad i \in I^{PFR}, \quad sk \in SK \\
F_{D_{m}, FR_{i,m}, MR_{i}, IN_{i}, OUT_{i}} &\geq 0 \\
RM_{i}, RFS_{i,sk,m}, MRS_{i,sk}, INS_{i,sk} &\geq 0 \\
OUTS_{i,sk}, RRS_{i,k,sk}, BP_{i,sk}, XFIN_{m} &\geq 0 \\
XIN_{m,i}, XOUT_{i,sk,m}, XINS_{i,sk,m}, XOUTS_{m,i} &\geq 0 \\
V_{i}, VS_{i,sk}, R_{rp,i}, RS_{rp,i,sk}, CN_{i,m}, CNS_{i,sk,m} &\geq 0 \\
Z_{i}, ZS_{i,sk} &\in \{0, 1\}.
\end{align*}
\]
Examples 3 & 5

\[ \frac{r_A}{r_B} = 0.25 \]

\[ r_C = 0.2 \text{ CA}^2 \]

\[ r_D = 0.4 \text{ CA}^2 \]

\[ V = 100 \text{ lit/min} \]

\[ C_{A0} = 1 \text{ mol/lit} \]

From CRE

\[ C_{A_{opt}} = \sqrt{\frac{k_0}{k_2}} \]

\[ k_0 = 0.025 \text{ lit/mol} \]

\[ k_2 = 0.25 \text{ lit/mol} \]

\[ \text{CA} \]

\[ \frac{C_{x}}{C_{l0}} = 0.5 \text{ mixed} \]

\[ V_{mixed} = 750 \text{ lit} \]

\[ C_{R} = 0.375 \text{ and} \]

\[ C_{R} = 0.375 \text{ and} \]
Example 3  Three different solutions

CES 45 595 (1990)
A $\xrightarrow{k_1} B \xrightarrow{k_2} C$

$V_1 < V_2 < V_3$

$53.02 \text{ kmol/hr}$

$47.98 \text{ kmol/hr}$

$50 \text{ kmol/hr}$

Use only PFRs

CES 46 1376 (1991)
A train of bubble columns (sparged reactors) through which liquid toluene and chlorinated products flow in series while chlorine is added into each column and hydrogen is removed from the column.

Typical selectivity to benzyl chloride: 90%  But Toluene conversion is less than 30%. Can one do better?

Process Intensification via Multifunctionality by Reaction – Separation Coupling: Proposed Technology Configured into a Semi-Batch Mode

Schematic of Photo Reactive Distillation System

Allows in situ product removal and toluene recycle.

Selectivity to benzyl chloride: 96% + up to toluene conversion of 98%.

Alkylation: HF Catalyst (Old); Deactivating Solid Supported Liquid Catalyst or Solid Acid Catalyst (New)

OLD REACTOR: MIXER-SETTLER WITH EXTERNAL RECYCLE PUMP

PRODUCT \( \bar{t} = 40 \text{ min} \)

HF RECYCLE with a pump !!

NEWER REACTOR: “LIFT” PRINCIPLE: NO RECYCLE PUMP

PRODUCT \( \bar{t} = 30 \text{ sec} \)

HF INTERNAL RECYCLE no pump !! no leaky seals !! Still HF is there!!

Simultaneous Development of Catalyst and Reactor Technology

Need reactor model to assess selectivity and productivity
Radioactive Particle Tracking (CARPT) Provides Solids Velocity and Mixing Information

Computer Tomography (CT) Provides Solids Density Distribution

Low Pressure Side (<80 psi)

Cold Flow Model

High Pressure Side (80-100 psi)

Tracer Studies Confirm Liquid In Plug Flow (N > 20) (Devanathan, 1990; Kumar, 1994; Roy, 2000)
CARPT Results

Comparison of CFD with Data

Final 2-D Convection Diffusion Reactor Model for the Riser

Ready for plant design, optimization and model based control.

Slow down of catalyst deactivation should be explored by CO2 addition at supercritical conditions.
Example 7
Denbigh reactions

\[
\begin{align*}
C_{A0} &= 6.0 \text{ mol/lit} \\
C_{B0} &= 0.6 \text{ mol/lit} \\
\nu &= 100 \text{ lit/hr}
\end{align*}
\]

\[
\begin{align*}
C_{A0} &= 6.0 \\
C_{B0} &= 0.6
\end{align*}
\] (plug flow)

\[
\nu = 20.706 \text{ lit}
\]

\[
\begin{align*}
A &\rightarrow B: n=2, k=1 \\
B &\rightarrow C: n=1, k=0.65^{-1} \\
B &\rightarrow D: n=1, k=0.65^{-1} \\
B &\rightarrow E: n=2, k=0.1
\end{align*}
\]

maximize \[
\frac{C_B}{C_D}
\]

\[
\frac{C_B}{C_D} = ?
\]

CES 45 595 (1990)
Computers can be very useful to solve tedious repetitive problems involving lots of ugly mathematics.

Don't discard general concepts. In the area of reactors they bring understanding.

Beware of... more powerful methods are naturally better.

Use common sense.
The reactor supermarket

- packed bed
- membrane reactor
- fluid bed
- circulating fluid bed
- slurry reactor
- bunker reactor
- catalytic distillation reactor
- MTBE
- methanol
- methanol, i-butene, n-butene
F. Cottrell (U.S. Patent, 1938)-Foul Gas Deodorizer

A Standard Reverse Flow Process

The temperature profile in a bi-directional FBR with an exothermic reaction

\( T_{\text{feed}} < T_{\text{bed,0}} \)

- An inverted U shaped temperature profile in a bi-directional FBR.
- Overcomes equilibrium limitations.
- Achieves high temperatures with dilute feed.

- Matros (1989)
- Van de Beld & Westerterp (1996)
- Eigenberger & Nieken (1988)
Asymmetric Reverse Flow Process
Wrong-Way Coupling (Kulkarni and Dudukovic (1996-1998))

Exo: Methanol combustion
Endo: Methane Steam Reforming

Traditional FBR is limited by dynamic and thermodynamic parameters and is inefficient and impractical for highly exothermic reactions
A SYSTEMS APPROACH TO MULTIPHASE REACTOR SELECTION

Economics

Reactants

Reactors Type & contacting pattern

Products

Process Requirements
• max: selectivity
• max: conversion
• max: productivity
• stable
• easy scale-up
• operability
• heat transfer

Environmental constraints
• minimum pollution
• energy efficiency

WHY SYSTEMS APPROACH?
• Number of configurations extremely large
• Limits to intuitive decision making
• Innovations are possible
Chemical Reaction Engineering Basics

- Molecular Level
  - Mechanisms and kinetic rates

- Eddy (Particle) Level
  - Micromixing & kinetics
  - Intra phase diffusional effects (Thiele modulus, effectiveness factor)
  - Inter phase transport effects

- Reactor Level
  - Ideal flow patterns (CSTR, PFR)
  - Non-ideal flow patterns between phases
  - Contacting patterns
  - Mixing
Multiphase Reactor Selection Methodology

I. Volume / Interfacial Area for the Phases
   ~ $d_p$ for gas-solid systems
   ~ $\beta$ for gas-liquid systems
   ~ $d_p$ and $\beta$ for G-L-S systems

II. Contacting & Flow Pattern
   a) RTD for each phase (PF, backmixed)
   b) Co – Counter – Cross current?
   c) • Split addition
      • Product removal in situ, etc.

III. Flow Regime
   • Homogeneous
   • Churn turbulent
   • Dense phase riser (air lift)
   • Dilute phase riser (spray)