SKF4153- PLANT DESIGN

PROCESS SYNTHESIS & CREATION

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SELECTION CRITERIA

- Thermo-physical property data
  - physical properties (T, P, conversion)
  - phase equilibria (VLE data)
  - Property prediction methods
- Environmental and safety data
  - toxicity data
  - flammability data
- Chemical Prices
  - e.g. as published in the *Chemical Marketing Reporter*
- Experiments
  - to check on crucial items above

} Knovel website, MSDS, NIST chemical webpage, patents, etc.

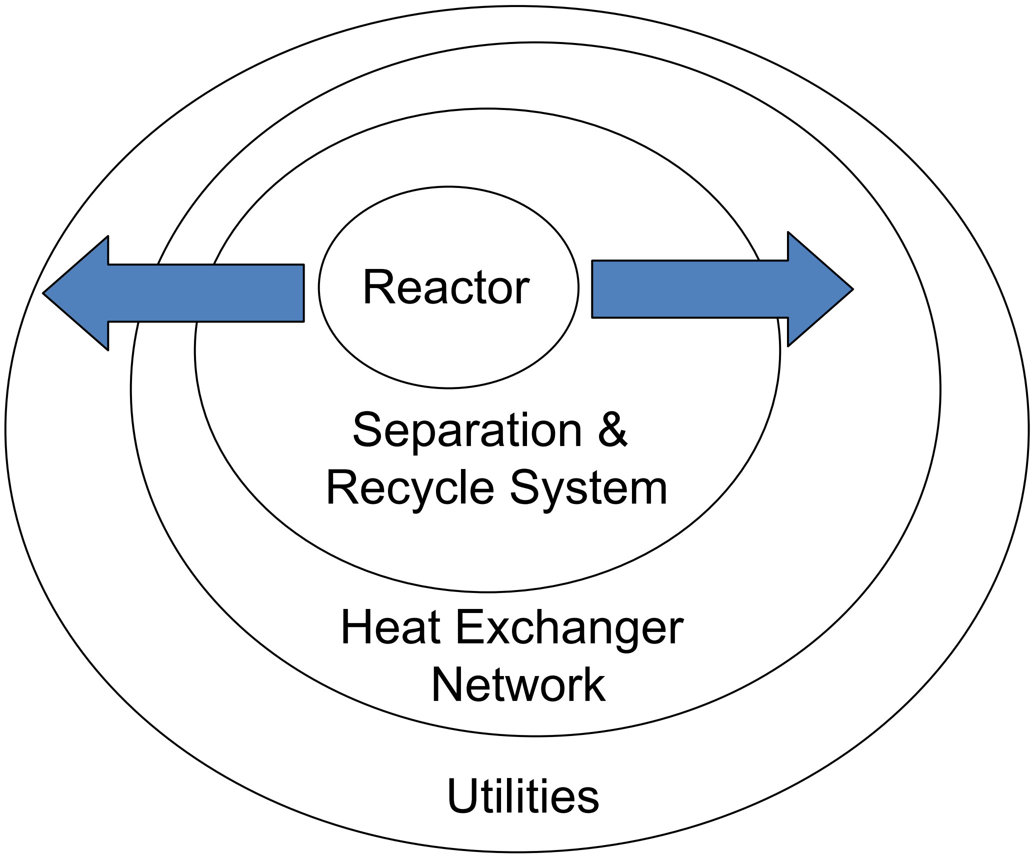
PROCESS SYNTHESIS

◎Synthesis steps (Rudd, Powers, Sirrola, 1973) -

- ❖Eliminate differences in molecular types (chemical reaction)
- ❖Distribute chemicals by matching *sources* and *sinks* (mixing & recycle)
- ❖Eliminate differences in composition (separation)
- ❖Eliminate differences in temperature, pressure and phase
- ❖Integrate tasks (combine *tasks* into *unit operations*)

Reference: W.D. Seider, J.D. Seider, D.R. Lewin, Product and Process Design Principles: Synthesis, Analysis and Evaluation, John Wiley and Sons, Inc., 2010.

The “Onion” Model (Smith and Linnhoff, 1995)



Synthesis Step 1:
Eliminate Differences in Molecular Types

Compare advantages and **disadvantages** of all type of reactions possible…

RECALL

IRREVERSIBLE	REVERSIBLE
Feed1 + Feed2 $\longrightarrow$ Product	Feed1 + Feed2 $\rightleftharpoons$ Product + Byproduct

IRREVERSIBLE

An excess of one feed component would force another feed component to complete conversion.

Which feed in excess ?

- Cost
- Safety

REVERSIBLE

Maximum conversion is limited by the equilibrium conversion

To increase equilibrium conversion:

- Adding access of one feed
- Remove byproduct

WHAT IF SIDE REACTION IS REVERSIBLE?

$$\text{Feed1} + \text{Feed2} \longrightarrow \text{Product} \quad \text{...............(1)}$$

$$\text{Feed1} + \text{Product} \rightleftharpoons \text{Byproduct} \quad \text{...............(2)}$$

TO MAXIMIZE SELECTIVITY,
INHIBIT THE BYPRODUCT FORMATION

By using <u>excess of Feed2</u> will force Feed1 to complete conversion and inhibit the side reaction

Or, removing the product as reaction proceed will force the secondary reaction to left side and inhibit the Byproduct formation

EXERCISE

- Benzene is produced from toluene,

$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

- Biphenyl, the unwanted byproduct is produced from benzene,

$2C_6H_6 \rightarrow C_{12}H_{10} + H_2$

- Calculate the conversion, selectivity and yield with respect to toluene.

	Inlet Flow (kmol/hr)	Outlet Flow (kmol/hr)
H_2	1858	1583
CH_4	804	1083
C_6H_6	13	282
$C_6H_5CH_3$	372	93
$C_{12}H_{10}$	0	4

GROSS PROFIT EVALUATION

- Monochlorodecane (MCD) $C_{10}H_{21}Cl$ is produced through,

$$C_{10}H_{22} + Cl_2 \rightarrow C_{10}H_{21}Cl + HCl$$

- A side reaction to which unwanted byproduct dichlorodecane (DCD) is produced

$$C_{10}H_{22} + 2Cl_2 \rightarrow C_{10}H_{20}Cl_2 + 2HCl$$

- Calculate E.P.
- What would you suggest to increase the production yield?

	Molecular weight	Price ($/kg)
HCl	36	0.35
Chlorine	71	0.21
DEC	142	0.27
MCD	176	0.45
DCD	211	0.00

Synthesis Step 2: Matching sources and sinks

How much **reactant** do we need to obtain the desired **production rate**? Can we recycle un-reacted reactant?

Synthesis Step 3:
Eliminate Differences in Composition

How to **separate** desired and undesired product? Can we **recycle** to obtain **higher production**?

To eliminate differences in composition, 2 distillation towers in series are inserted. Distillation is desirable because of large volatility differences among the 3 species.

See the boiling points in table below.

	Boiling point (°C)				Critical constants	
Chemical	1 atm	4.8 atm	12 atm	26 atm	T_c, °C	P_c, atm
HCl	-84.8	-51.7	-26.2	0	51.4	82.1
C_2H_3Cl	-13.8	33.1	70.5	110	159	56
$C_2H_4Cl_2$	83.7	146	193	242	250	50

Synthesis Step 4:
Eliminate Differences in T, P and Phase

Identify all **T, P and phase change** to determine the required **utility systems**…

How do we set the T and P?

Sensible operating range to avoid severe processing difficulties

Parameter	Range	**Rationale**
Pressure	Between 1 to 10 bar	Most equipment can go up to 10 bar without increase in capital cost
Temperature	40 to 260°C	Limited by utilities available: cooling water @ (30°C) and steam between 40 to 60 bar (260°C)

Pressure Range

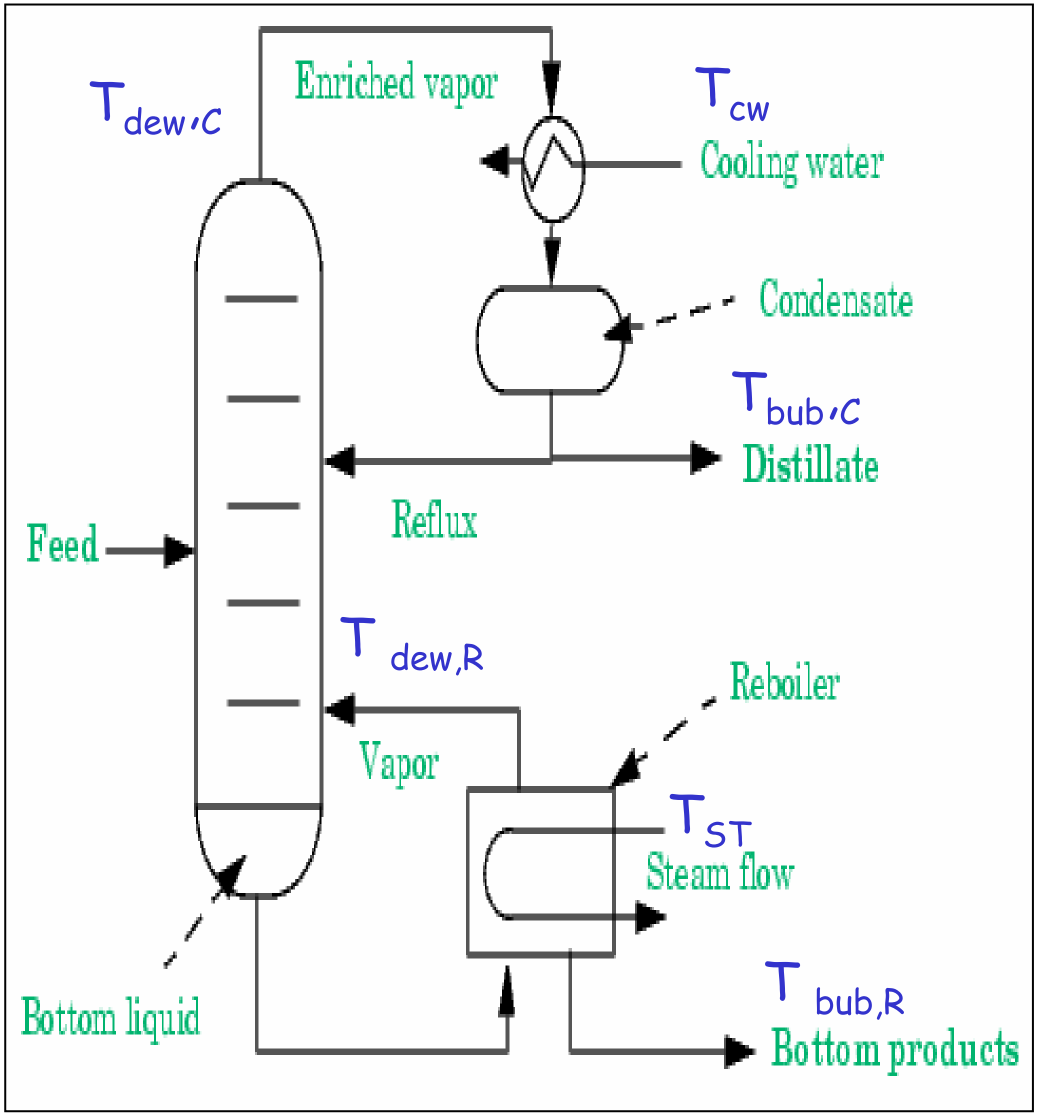
The decision to operate outside the range of 1 to 10 bar usually is a compromise between performance and the capital and operating costs of process equipment.

Conditions	Justification	**Penalty**
P > 10 bar	In gas operations, increased density, lower volume, smaller equipment (for the same residence time), higher quality heating media (steam)	More costly, thicker-walled equipment needed
P < 1 bar	Prevent degradation of heat-sensitive materials	Larger equipment. Need special equipment construction for vacuum operations

Column Temperature

Primarily dictated by cooling water temp., Tcw :

$T_{CW} \leq T_{bub,C} \leq T_{dew,C} \leq T_{bub,R} \leq T_{dew,R} \leq T_{ST}$



Synthesis Step 5:
Integrate Tasks

Complete the **unit operations**…

Process Equipment Identification

Process Equipment	General Format XX-YZZ A/B
	XX are the identification letters for the equipment classification
	C - Compressor or Turbine
	E - Heat Exchanger
	H - Fired Heater
	P - Pump
	R - Reactor
	T - Tower
	TK - Storage Tank
	V - Vessel
	Y designates an area within the plant
	ZZ is the number designation for each item in an equipment class
	A/B identifies parallel units or backup units not shown on a PFD
Supplemental Information	Additional description of equipment given on top of PFD

Consider P-101A/B:

P-101A/B identifies the equipment as a **Pump**
P-**1**01A/B indicates that the pump is located in **Area 100** of the plant
P-1**01**A/B indicates that this specific pump is **number 01** in Area 100
P-101**A/B** indicates that a **back-up pump** is installed. Thus, there are two identical pumps, P-101A and P-101B. One pump will be operating while the other is idle.

EXERCISE

- Monochlorodecane (MCD) $C_{10}H_{21}Cl$ is produced through,

$C_{10}H_{22} + Cl_2 \rightarrow C_{10}H_{21}Cl + HCl$

- A side reaction to which unwanted byproduct dichlorodecane (DCD) is produced

$C_{10}H_{22} + 2Cl_2 \rightarrow C_{10}H_{20}Cl_2 + 2HCl$

- Develop a process flowsheet according the 5 synthesis steps.

B.P @ 1 atm	Molecular weight	Boiling Pt. (K)
HCl	36	188
Chlorine	71	239
DEC	142	447
MCD	176	488
DCD	211	495

Assume:

- Incomplete conversion of both feed.
- Reaction at 152 K, 2 atm.
- Feed to the first separation is at 200K, 10 atm.

SUMMARY

Key information (materials and products)

- Thermo-physical property data
- Environmental and safety data
- Chemical Prices
- Batch or continuous operations
- Unit operations involved

Key steps in designing a process plant

- Chemical reaction
- Mixing & recycle
- Separation processes
- Eliminate differences in temperature, pressure and phase
- Integrate tasks (combine *tasks* into *unit operations*)

References

- J.M. Coulson, J.F. Richardson, R.K. Sinnot, Chemical Engineering Vol. 6, Pergamon Press, 1985.
- J.M. Douglas, Conceptual Design of Chemical Processes, McGraw Hill, 1998.
- L.T. Biegler, I.E. Grossman, A.W. Westerberg, Systematic Methods of Chemical Process Design, Prentice Hall, 1997.
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