Seider/Seader/Lewin: Product and Process Design Principles
Chapter 5

Heuristics for Process Synthesis

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Design teams use heuristics when generating alternatives that make up a synthesis tree

Heuristics for Process Synthesis

- This lecture deals with the heuristic rules that expedite the selection and positioning of processing operations as flowsheets are assembled.

- These rules are based on experience and hold in general, but should be tested (e.g., by simulation) to ensure that they apply in the specific application.

Heuristics for Process Synthesis

When you have finished studying this unit, you should:

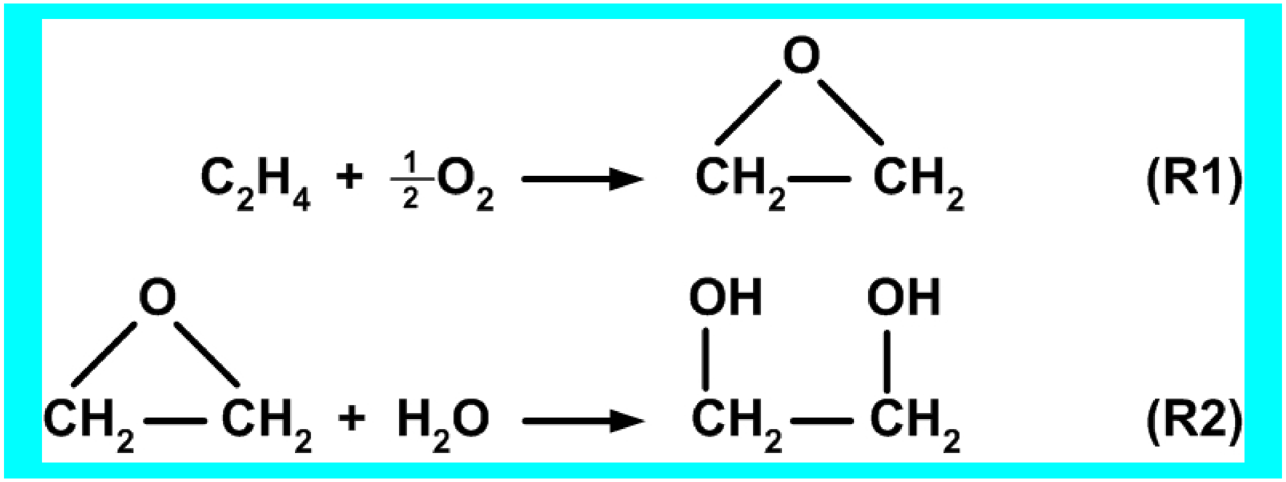
- Understand the importance of selecting reaction paths that do not involve toxic or hazardous chemicals, and when unavoidable, to reduce their presence by shortening residence times in the process units and avoiding their storage in large quantities.
- Be able to distribute the chemicals in a process flowsheet, to account for the presence of inert species, to purge species that would otherwise build up to unacceptable concentrations, to achieve a high selectivity to the desired products.
- Be able to apply heuristics in selecting separation processes to separate liquids, vapors, and vapor-liquid mixtures.
- Be able to distribute the chemicals, by using excess reactants, inert diluents, and cold shots, to remove the exothermic heats of reaction.
- Understand the advantages of pumping a liquid rather than compressing a vapor.

Raw Materials and Chemical Reactions

Heuristics 1

Select raw materials and chemical reactions to avoid, or reduce, the handling and storage of hazardous and toxic chemicals.

- **Example:** Manufacture of Ethylene Glycol (EG).



Since both reactions are highly exothermic, they need to be controlled carefully. But *a water spill into an ethylene-oxide storage tank could lead to an accident similar to the Bhopal incident.* Often such processes are designed with two reaction steps, with storage of the intermediate, to enable continuous production, even when maintenance problems shut down the first reaction operation.

Raw Materials and Chemical Reactions

Heuristics 1

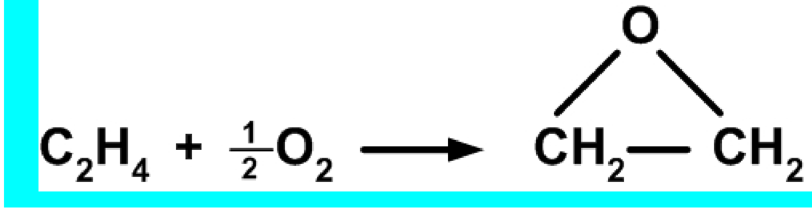
Alternatives to the two-step EG process

- **Alternative 1:** Use costly chlorine and caustic in a single reaction step, to avoid the intermediate:

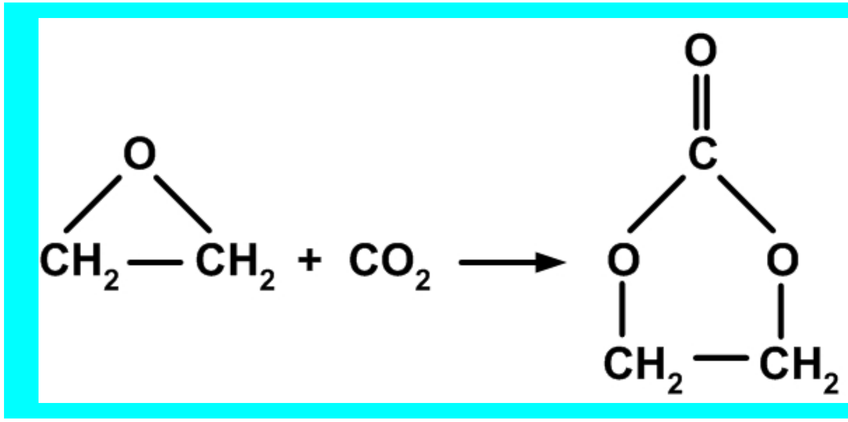
$$C_2H_4 + Cl_2 + 2NaOH_{(aq)} \longrightarrow \overset{OH}{\overset{|}{CH_2}} - \overset{OH}{\overset{|}{CH_2}} + 2NaCl$$

(R2)

- **Alternative 2:** As ethylene-oxide is formed, react it with carbon dioxide to form ethylene-carbonate, a much less active intermediate that can be stored safely and hydrolyzed, to form the ethylene-glycol product, as needed:



(R1)



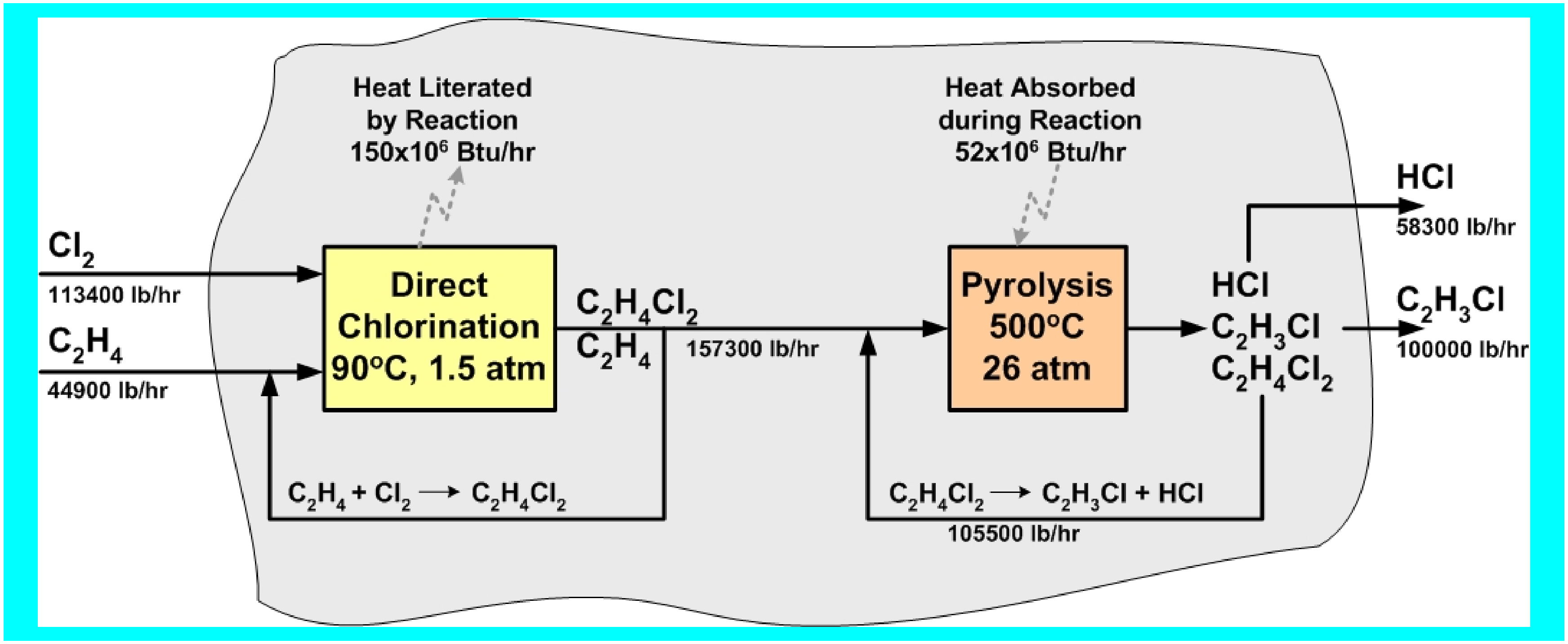
(R4)

Distribution of Chemicals

Heuristics 2

Use an excess of one chemical reactant in a reaction operation to completely consume a second valuable, toxic, or hazardous chemical reactant.

- **Example:** Using excess ethylene in dichloroethane (→ vinyl chloride) production to consume completely the hazardous and toxic chlorine (**Q:** ethylene/chlorine ratio ?)

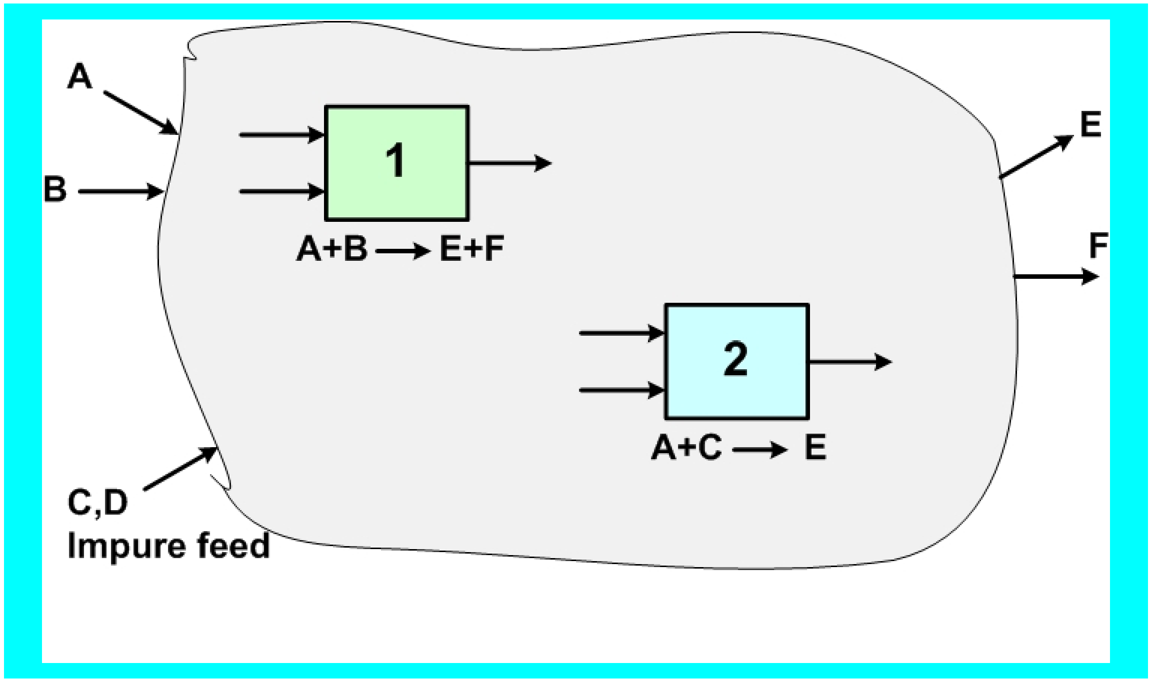


Distribution of Chemicals

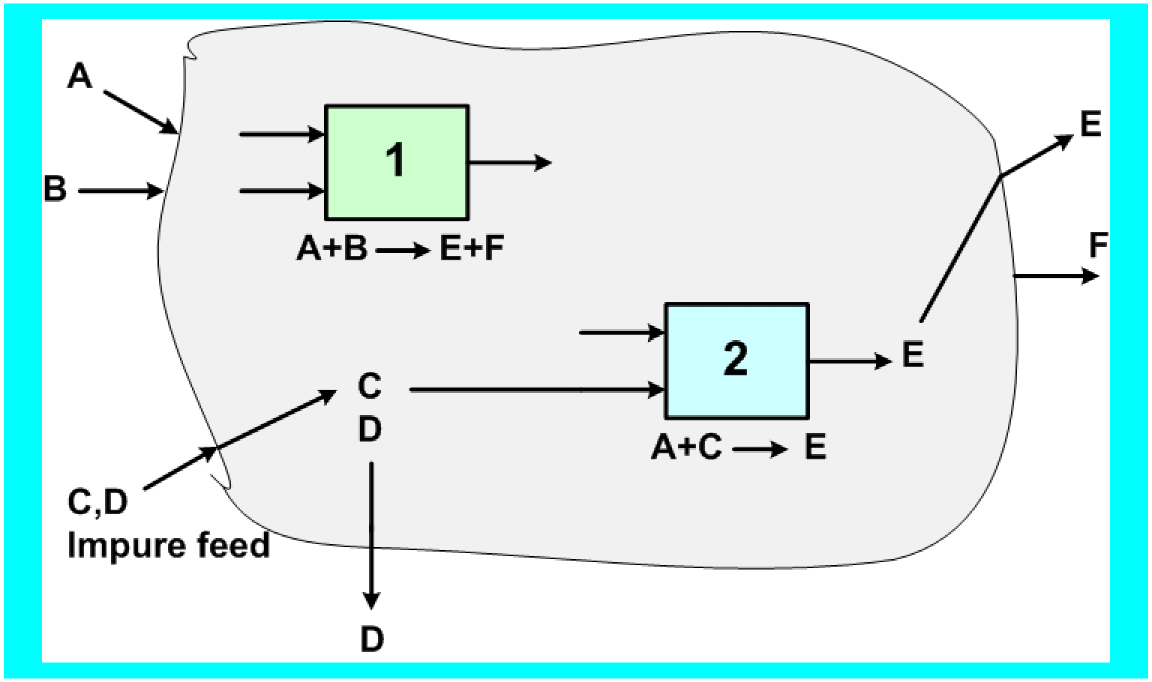
Heuristics 3

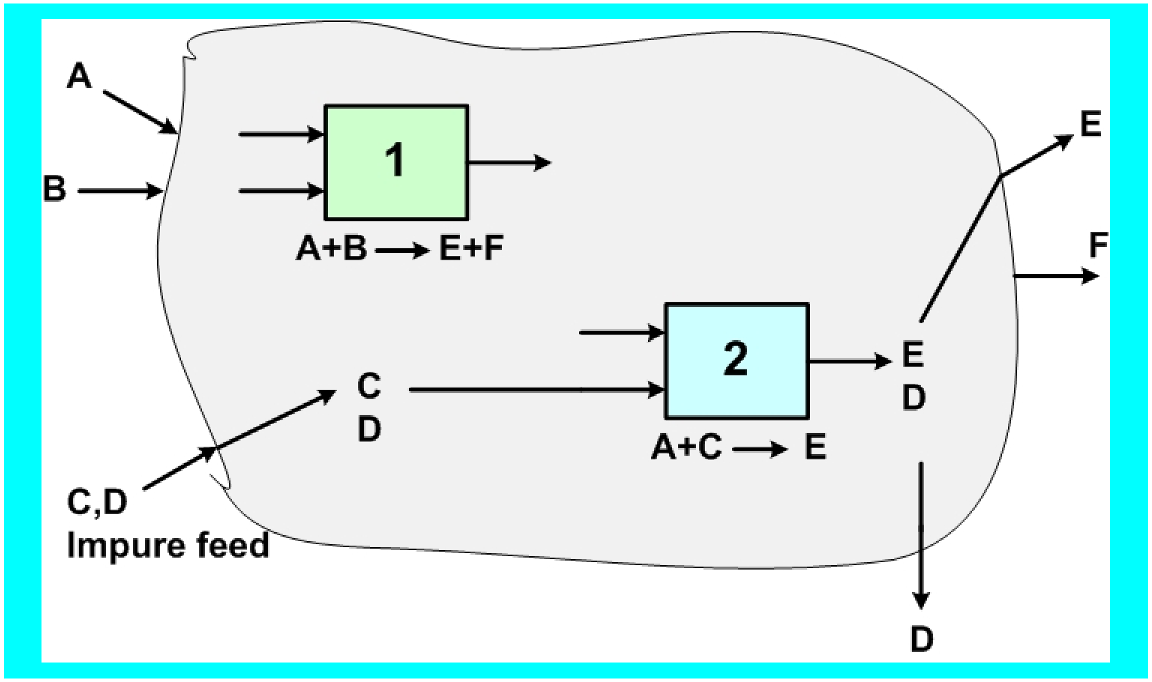
Inert Species: When nearly pure products are required, eliminate inert species before the reaction operations, when the separations are easily accomplished, or when the catalyst is adversely affected by the inert.

Do not do this when a large exothermic heat of reaction must be removed.

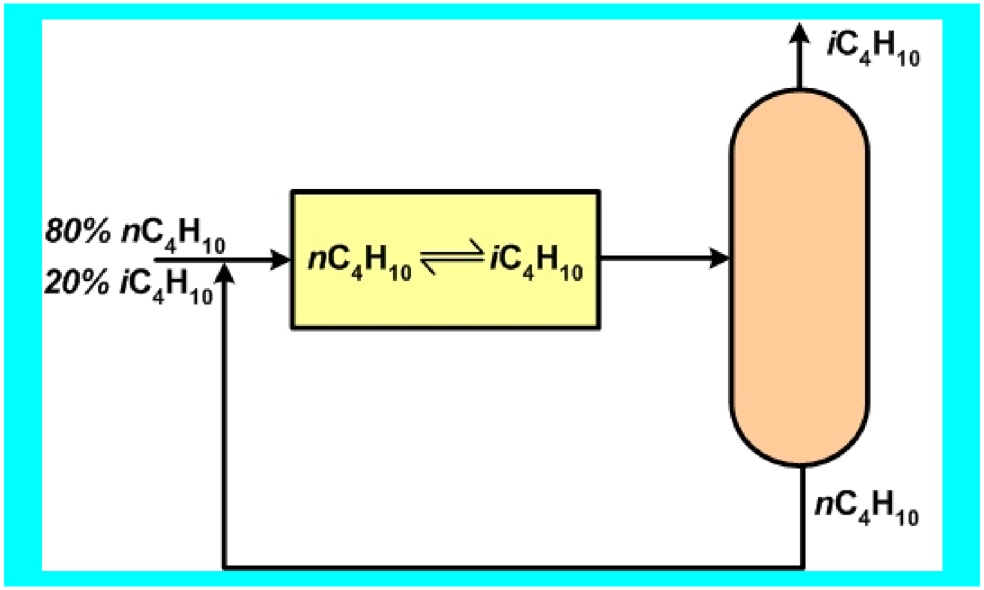


Distribution of Chemicals

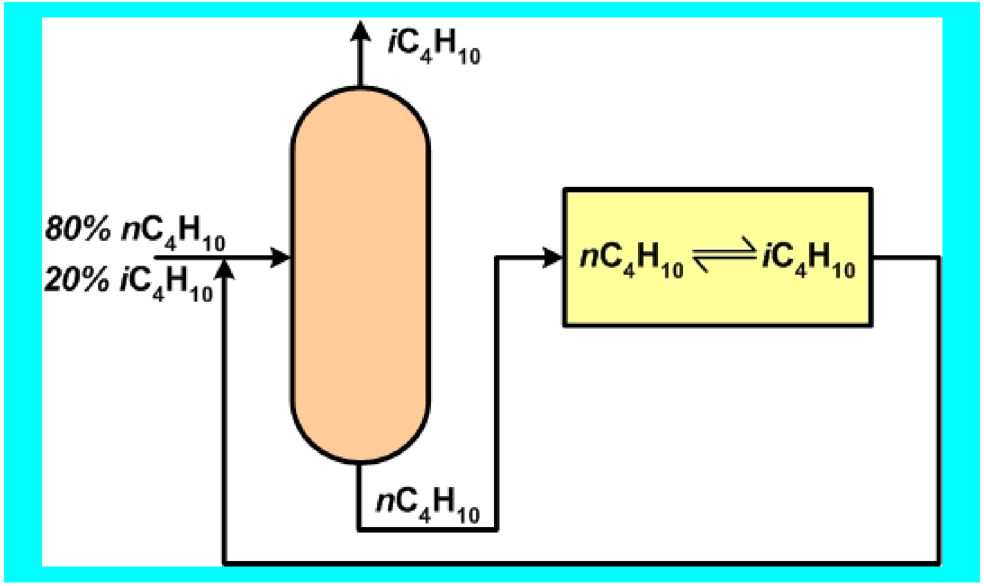




Distribution of Chemicals



By positioning the distillation column first, a nearly pure feed is sent to the reaction operation, providing a higher conversion to *iso*-butane.



Distribution of Chemicals

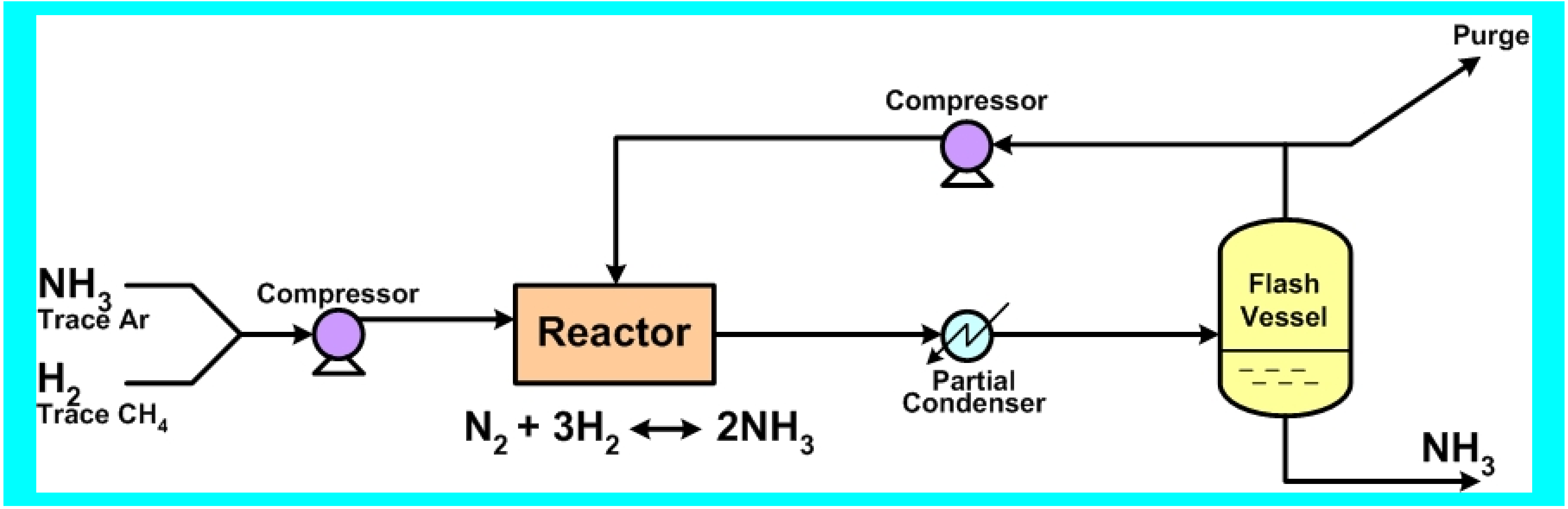
Heuristics 4

Purge Streams: Introduce liquid or vapor purge streams to provide exits for species that

- enter the process as impurities in the feed
- produced by irreversible side-reactions

when these species are in trace quantities and/or are difficult to separate from the other chemicals. Lighter species leave in vapor purge streams, and heavier species exit in liquid purge streams.

Example: NH3 Synthesis Loop.



Note: Purge flow rate selection depends on economics!

Distribution of Chemicals

Heuristics 4

- **Example: Ammonia Process Purge**
  The ammonia reactor loop is simulated to examine the effect of purge-to-recycle ratio on the compositions and flow rates of the purge and recycle streams. The following specifications are made:

Simulation Unit	T (^{o}F)	P (atm)
R1	932	200
F1	-28	136.3

The combined feed stream, at 77^oF and 200 atm, is comprised of

	lbmol/hr	Mole Fraction
N_2	$24.$	0.240
H_2	74.3	0.743
Ar	0.6	0.006
CH_4	1.1	0.011
	100.0	1.000

Distribution of Chemicals

Heuristics 4

- **Example: Ammonia Process Purge**
  Several variables are tabulated as a function of the purge/recycle ratio:

Purge/Recycle Ratio	PROD Flow Rate (lbmole/hr)	Recycle Flow Rate (lbmole/hr)	Purge Flow Rate (lbmole/hr)	Purge mole Fraction Ar	Purge Mole Fraction CH_4
0.1	39.2	191.0	19.1	0.028	0.052
0.08	40.75	209.3	16.7	0.033	0.060
0.06	42.4	233.9	14.0	0.040	0.074
0.04	44.3	273.5	10.9	0.053	0.093
0.02	45.8	405.6	8.1	0.072	0.133

In all cases, the mole fraction of Ar and CH_4 in the purge are significantly greater than in the feed. As the purge/recycle ratio is decreased, the vapor effluent from the flash vessel becomes richer in the inert species and less H_2 and N_2 are lost in the purge stream. However, this is accompanied by a significant increase in the recycle rate and the cost of recirculation, as well as the reactor volume. The capital and operating costs should be estimated and a profitability measure should be optimized as a function of the purge/recycle ratio.

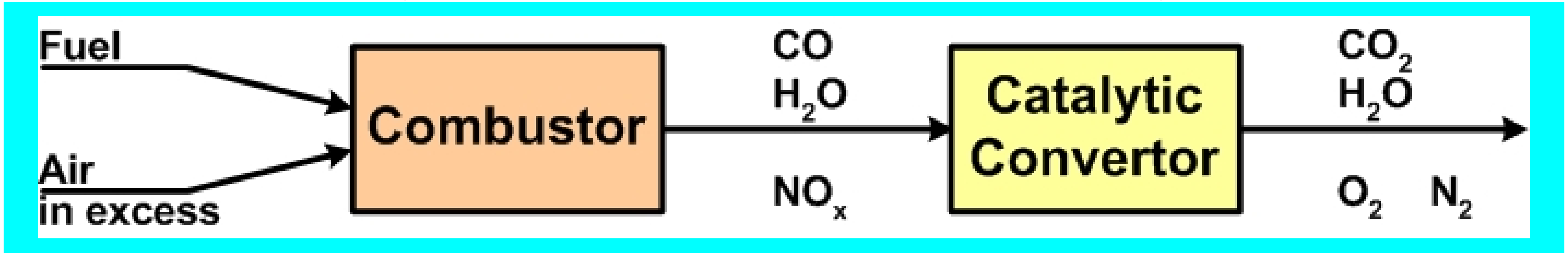
Distribution of Chemicals

Heuristics 5

Do not purge valuable species or species that are toxic and hazardous, even in small concentrations.

- ☞ Add separators to recover valuable species.
- ☞ Add reactors to eliminate toxic and hazardous species.

Catalytic converter in car exhaust system



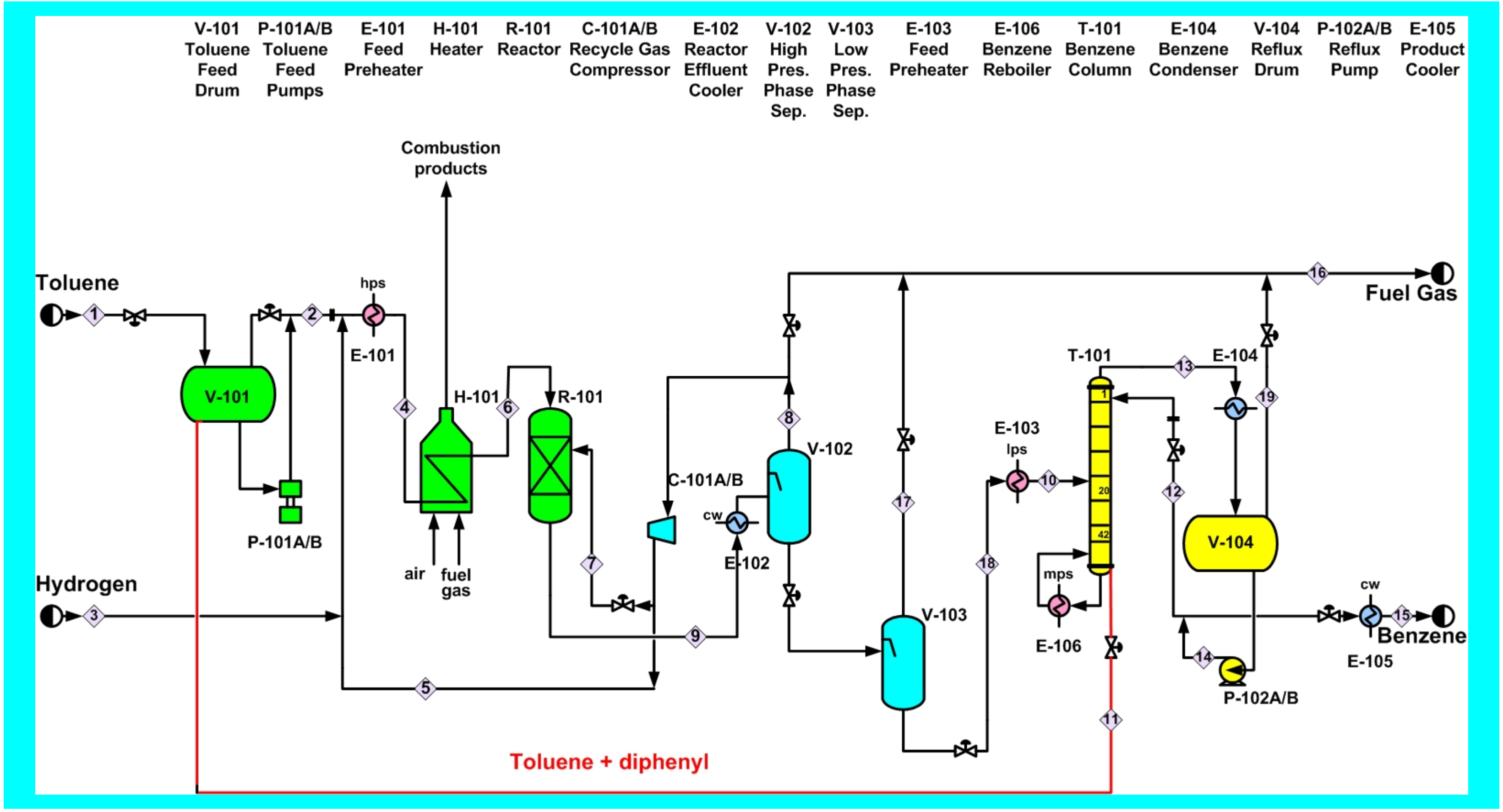
Distribution of Chemicals

Heuristics 6

Byproducts that are produced in reversible reactions, in small quantities, are usually not recovered in separators or purged. Instead, they are usually **recycled to extinction**.

- **Example: Reversible Production of Biphenyl** in toluene hydrodealkylation process

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

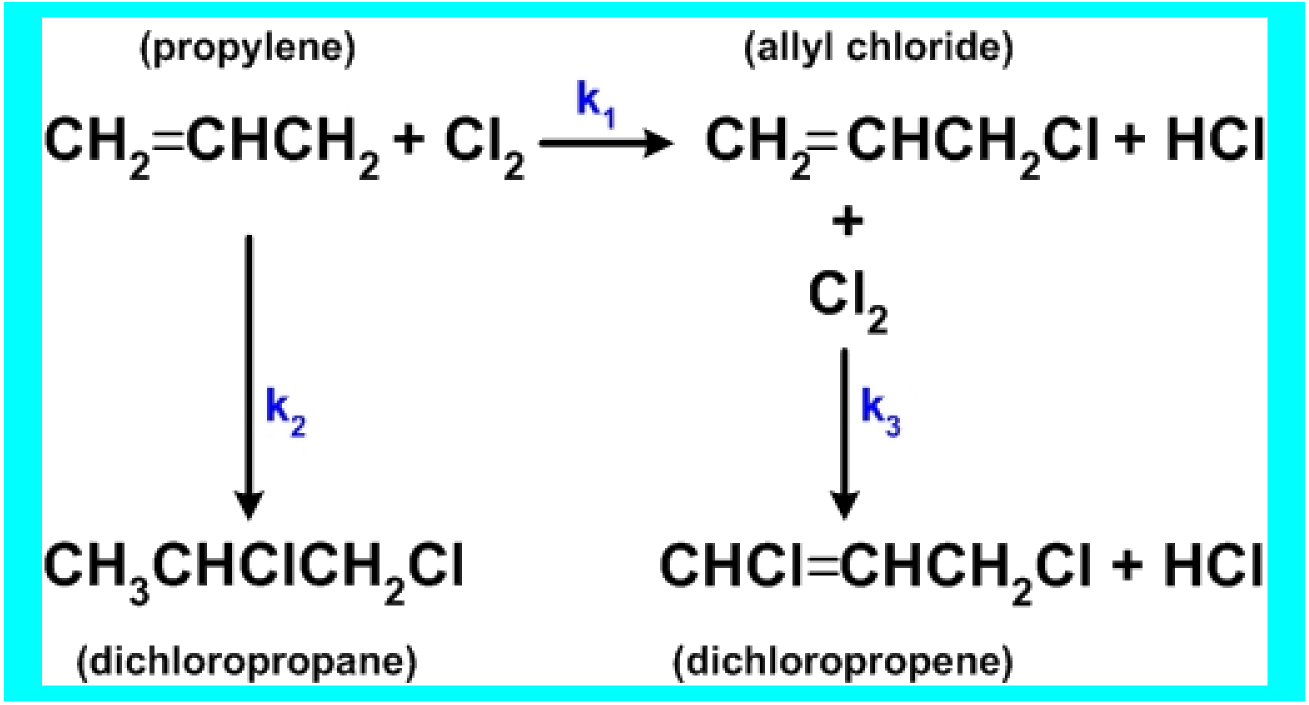


Distribution of Chemicals

Heuristics 7

For competing series or parallel reactions, adjust the temperature, pressure, and catalyst to obtain high yields of the desired products. In the initial distribution of chemicals, assume that these conditions can be satisfied - obtain kinetics data and check this assumption before developing a *base-case design*.

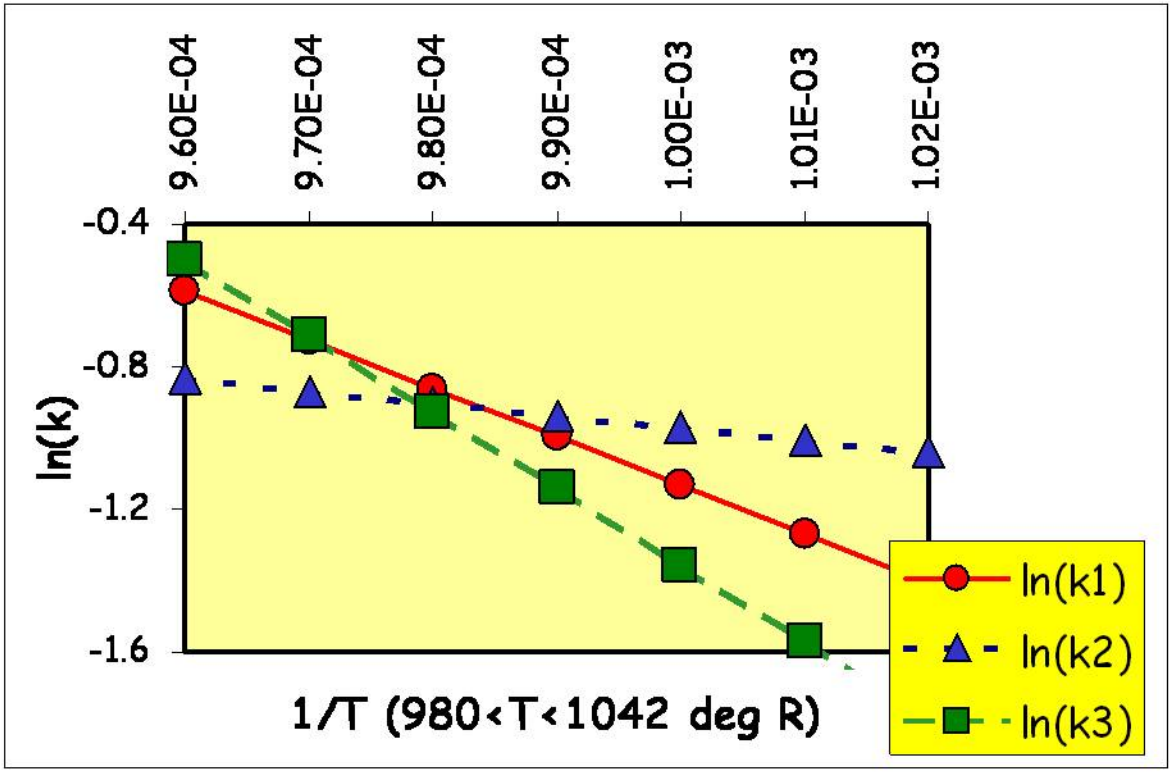
Manufacture of allyl-chloride



Manufacture of allyl-chloride: Kinetic Data

Reaction	ΔH_R Btu/lb-mole	k_o lb-mole/(hr ft^{3}atm^2)	E/R ^{o}R
1	$-4,800$	$206,000$	$13,600$
2	$-79,200$	11.7	$3,430$
3	$-91,800$	4.6×10^8	$21,300$

What range of operating temperatures favor production of Allyl Chloride ?



Distribution of Chemicals

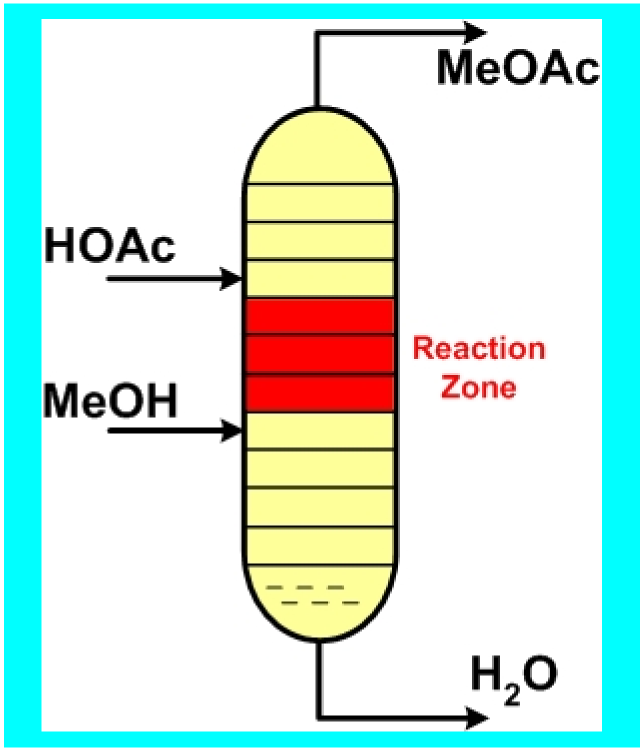
Heuristics 8

For reversible reactions, especially, consider conducting them in a separation device capable of removing the products, and hence, driving the reactions to the right. Such reaction-separation operations lead to very different distributions of chemicals.

- **Example:**
  Manufacture of Ethyl-acetate
  using reactive distillation.
  Conventionally, this would call for reaction:

  $$MeOH + HOAc \rightleftharpoons MeOAc + H_2O$$

  followed by separation of products using a sequence of separation towers.



Separations

Heuristics 9

Separate liquid mixtures using distillation and stripping towers, and liquid-liquid extractors, among similar operations, and so on, with the unreacted chemicals recovered in a liquid phase and recycled to the reaction operation.

Heuristics 10

Attempt to (partially) condense vapor mixtures with cooling water (typically to 35^oC) or a refrigerant. Then, use **Heuristic 9**.
Vapor/liquid purges are added when necessary to remove inerts that concentrate in the vapor/liquid and are not readily separated.

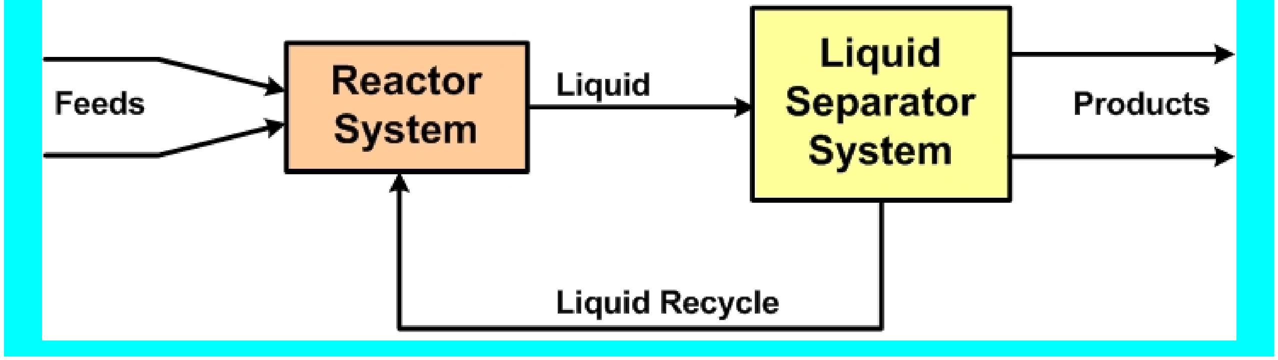
Heuristics 11

Separate vapor mixtures using partial condensers, cryogenic distillation, absorption towers, adsorbers, membrane devices.

Separations

Heuristics 9-11

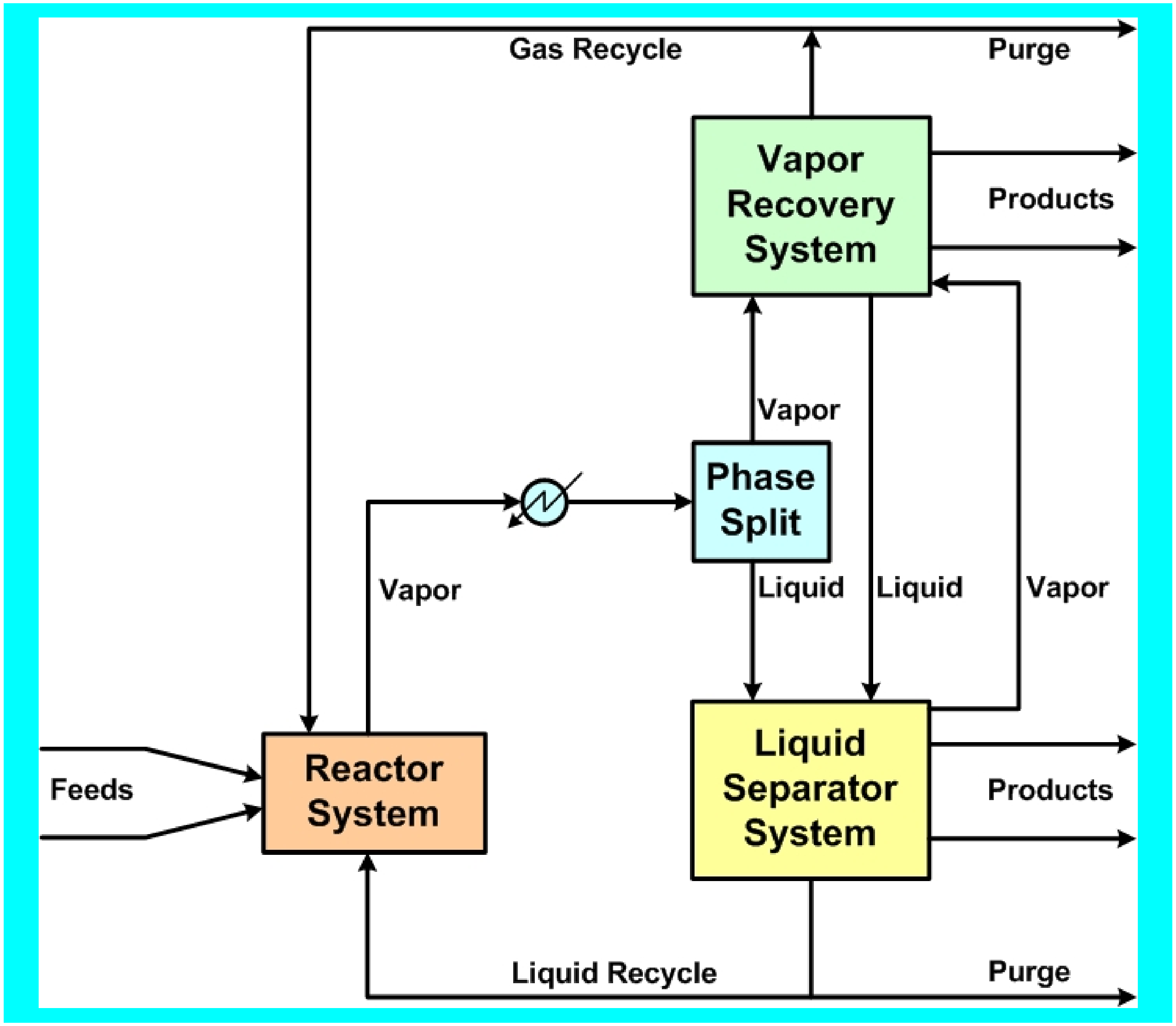
Flowsheet to separate liquid reactor effluents



Separations

Heuristics 9-11

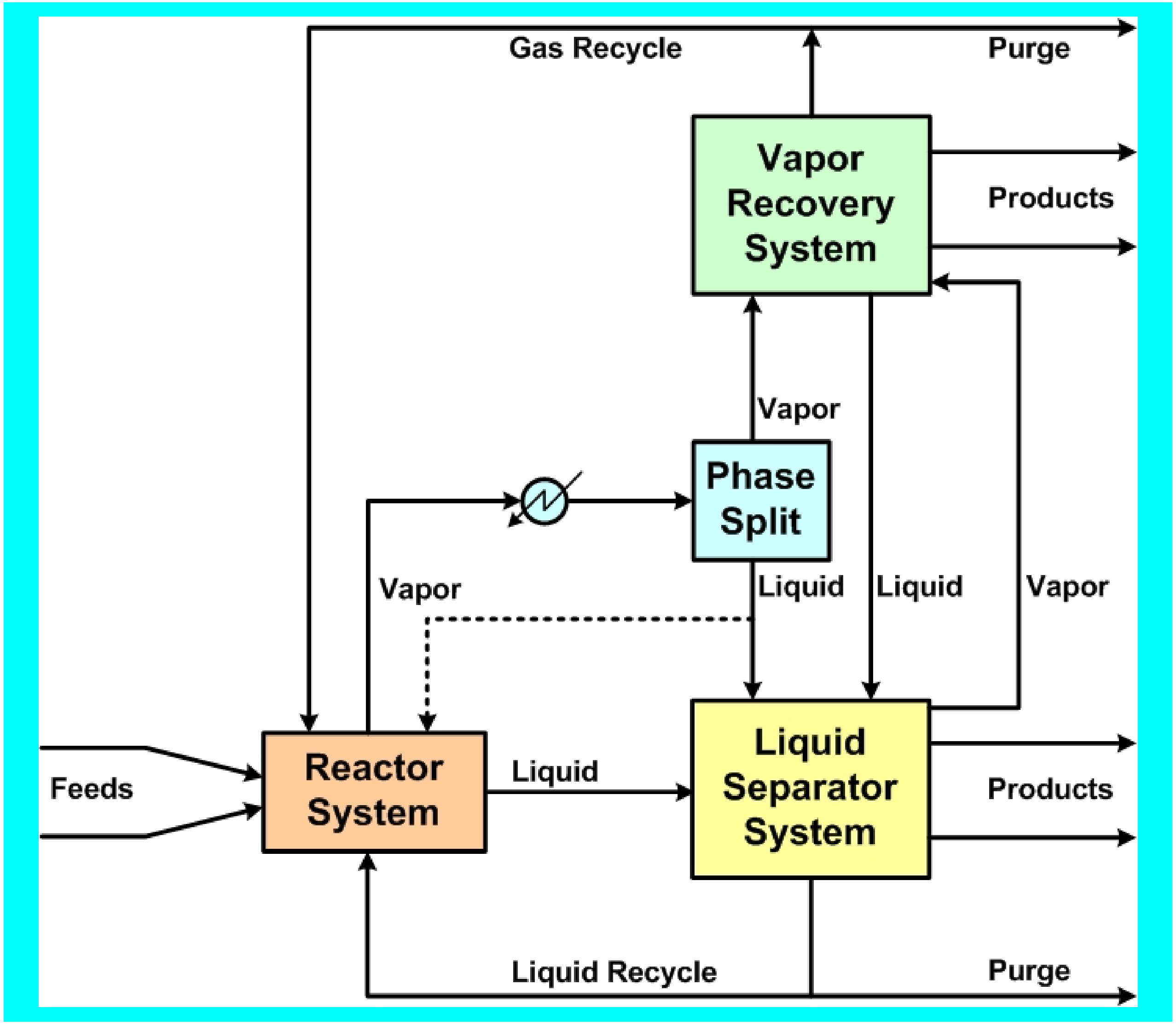
Flowsheet to separate vapor reactor effluents



Separations

Heuristics 9-11

Flowsheet to separate vapor/liquid reactor effluents



Separation Operations

— involving solid particles

- **Crystallization** occurs in three different modes:
  - ☞ *Solution Crystallization* applies mainly to inorganic chemicals, which are crystallized from a solvent (often water) with an operating temperature far below the melting point of the crystals.
  - ☞ *Precipitation* is fast solution crystallization that produces large numbers of very small crystals.

    It usually refers refers to the case where one product of two reacting solutions is a solid of low solubility (e.g., precipitation of insoluble silver chloride when aqueous solutions of silver nitrate and sodium chloride are mixed together).
  - ☞ In *Melt Crystallization*, two or more chemicals of comparable melting points are separated at an operating temperature in the ranges of melting temperatures (e.g., production of pure silicon wafers from a melt consisting of SiO_2).
- **Crystallization** is capable of producing very pure chemicals when conducted according to the following **heuristics**:

Separation Operations
— involving solid particles

Heuristics 12

Crystallize inorganic chemicals from a concentrated aqueous solution by chilling when solubility decreases significantly with decreasing temperature. Keep the solution at most 1 to 2^oF below the saturation temperature at the prevailing concentration.

Use crystallization by evaporation, rather than chilling, when solubility does not change significantly with temperature.

Separation Operations
— involving solid particles

Heuristics 13

Crystal growth rates are approximately the same in all directions, but crystals are never spheres. Crystal growth rates and sizes are controlled by limitlllg the extent of supersaturation.

$S = C/C_{\text{saturation}}$, where C is concentration, usually in the range $1.02 < S < 1.05$.

Growth rates are influenced greatly by the presence of impurities and of certain specific additives that vary from case to case.

Separation Operations

— involving solid particles

Heuristics 14

Separate organic chemicals by melt crystallization with cooling, using suspension crystallization, followed by removal of crystals by settling, filtration, or centrifugation. Alternatively, use layer crystallization on a cooled surface, with scraping or melting to remove the crystals. If the melt forms a solid solution instead of a eutectic, use repeated melting and freezing steps, called fractional melt crystallization, or zone melting to obtain nearly pure crystalline products.

Separation Operations
— involving solid particles

- Prior to crystallization, it is common to employ evaporation to concentrate a solution, particularly an aqueous solution of inorganic chemicals.

- Because of the relatively high cost of evaporating water with its very large heat of evaporation, the following heuristics are useful for minimizing the cost.

Separation Operations
— involving solid particles

Heuristics 15

Using multiple evaporators (called effects) in series, the latent heat of evaporation of water is recovered and reused. With a single evaporator, the ratio of the amount of water evaporated to the amount of external steam supplied to cause the evaporation is typically 0.8. For two effects, the ratio becomes 1.6; for three effects 2.4, and so forth. The magnitude of the boiling point elevation caused by the dissolved inorganic compounds is a controlling factor in selecting the optimal number of effects. The elevation is often in the range of 3 to 10^oF between solution and pure water boiling points. When the boiling point rise is small, minimum evaporation cost is obtained with 8 to 10 effects. When the boiling-point rise is appreciable, the optimal number of effects is small, 6 or less. If necessary, boost interstage steam pressures with steam-jet or mechanical compressors.

Separation Operations
— involving solid particles

Heuristics 16

When employing multiple effects, the liquid and vapor flows may be in the same or different directions.

Use forward feed, where both liquid and vapor flow in the same direction, for a small number of effects, particularly when the liquid feed is hot.

Use backward feed, where liquid flows in a direction opposite to vapor flows, for cold feeds and/or a large number of effects.

With forward feed, intermediate liquid pumps are not necessary, whereas they are for backward feed.

Separation Operations

— involving solid particles

- **Solution Crystallization** produces a slurry of crystals and mother liquor, which is partially separated by filtration or centrifugation into a wet cake and a mother liquor.
  - ☞ Filtration through a filter medium of porous cloth or metal may be carried out under gravity, vacuum, or pressure.
  - ☞ Centrifugation may utilize a solid bowl or a porous bowl with a filter medium.
- Important factors in the selection of equipment include:

  (1) moisture content of the cake, (2) solids content of the mother liquor,

  (3) fragility of the crystals, (4) crystal particle size, (5) need for washing the crystals to replace mother liquor with pure water, and (6) filtration rate.
- Filtration rate is best determined by measuring the rate of cake thickness buildup using a small-scale laboratory vacuum leaf filter test with the following criteria:

  Rapid, 0.1 to 10 cm/s; Medium, 0.1 to 10 cm/min; Slow, 0.1 to 10 cm/hr.

Separation Operations
— involving solid particles

Heuristics 17

When crystals are fragile, effective washing is required, and clear mother liquor is desired, use gravity, top-feed horizontal pan filtration for slurries that filter at a rapid rate; vacuum rotary drum filtration for slurries that filter at a moderate rate; and pressure filtration for slurries that filter at a slow rate.

Heuristics 18

When cakes of low moisture content are required, use solid-bowl centifugation if solids are permitted in the mother liquor, centrifugal filtration if effective washing is required.

Separation Operations
— involving solid particles

- Wet cakes from filtration or centrifugation operations are sent to dryers for removal of remaining moisture.

  A large number of different types of commercial dryers have been developed to handle the many different types of feeds, which include not only wet cakes, but also pastes, slabs, films, slurries, and liquids.

- The heat for drying may be supplied from a hot gas in direct contact with the wet feed or it may be supplied indirectly through a wall.

- Depending on the thickness of the feed and the degree of agitation, drying times can range from seconds to hours.

- The following heuristics are useful in making a preliminary selection of drying equipment.

Separation Operations
— involving solid particles

Heuristics 19

For granular material, free flowing or not, of particle sizes from 3 to 15 mm, use continuous tray and bell dryers with direct heat.

For free-flowing granular solids that are not heat sensitive, use an inclined rotary cylindrical dryer, where the heat may be supplied directly from a hot gas or indirectly from tubes, carrying steam, that run the length of the dryer and are located in one or two rings concentric to and located just inside the dryer rotating shell.

For small, free-flowing particles of 1 to 3 mm in diameter, when rapid drying is possible, use a pneumatic conveying dryer with direct heat.

For very small free-flowing particles of less than 1 mm in diameter, use a fluidized-bed dryer with direct heat.

Separation Operations

— involving solid particles

Heuristics 20

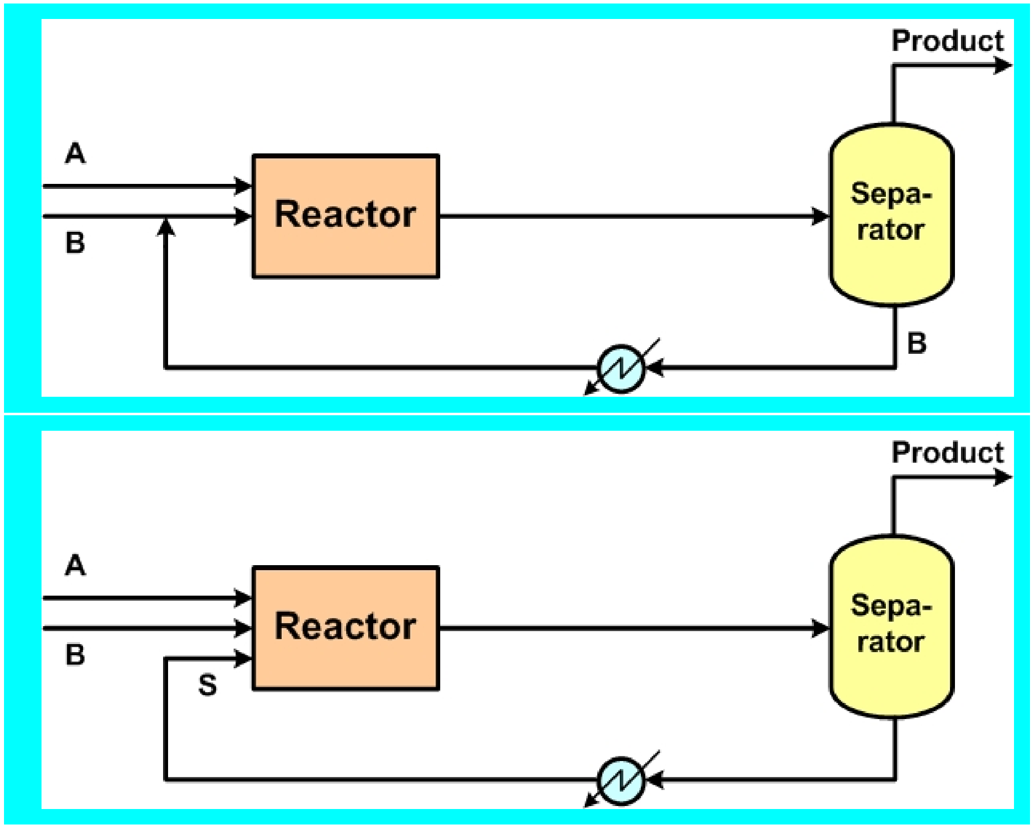
For pastes and slurries of fine solids, use a drum dryer with indirect heat.

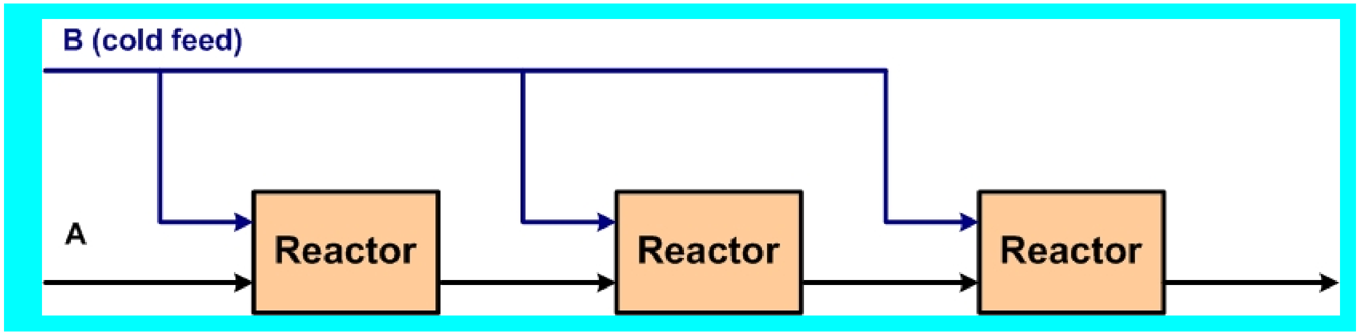
For a liquid or pumpable slurry, use a spray dryer with direct heat.

Heat Transfer in Reactors

Heuristics 21

To remove a highly-exothermic heat of reaction, consider the use of excess reactant, an inert diluent, and cold shots. These affect the distribution of chemicals and should be inserted early in process synthesis.





Heat Transfer in Reactors

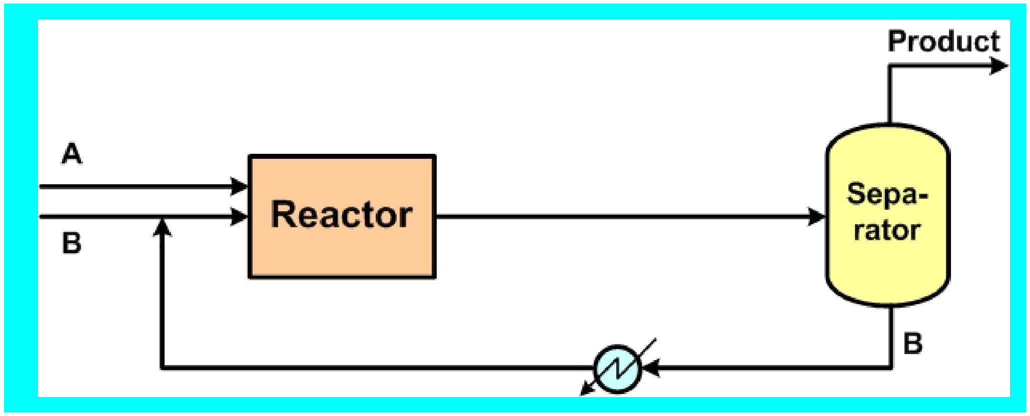
Heuristics 21

- **Example: Excess Reactant**
  Consider the reaction of carbon monoxide and hydroen to form methanol:

$$CO + 2H_2 \rightarrow CH_3OH$$

With the reactants fed in stoichiometric amounts at 25^oC and 1 atm, the “adiabatic reaction temperature” (complete reaction, zero heat duty, pressure of methanol product stream is returned to 1 atm) will be 1158^oC, which is far too high for the Cu-based catalyst and the materials of construction in most reactor vessels. Hence, a key question in the synthesis of methanol process, and similar processes involving highly exothermic reactions, is *how to lower the product temperature*.

Now suppose an excess of H_2 is specified such that the mole ratio of H_2/CO is arbitrarily 10 , then, with a complete conversion of CO, the effluent temperature will be reduced to 337^oC.



Heat Transfer in Reactors

Heuristics 21

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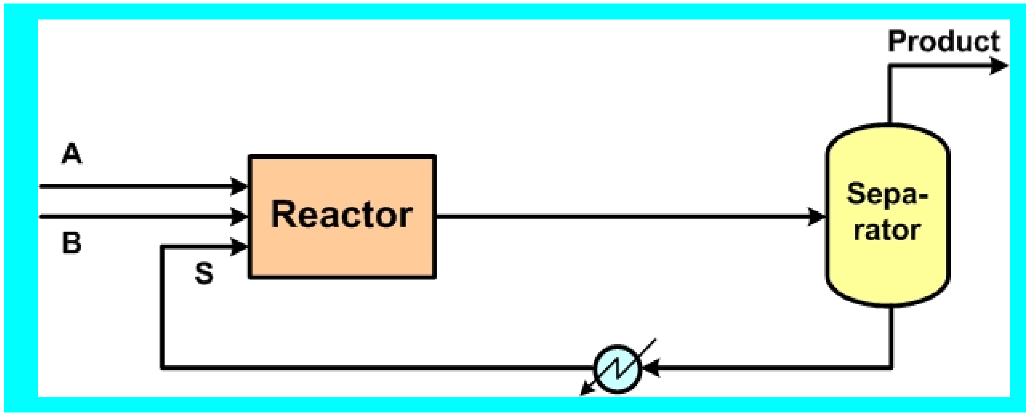
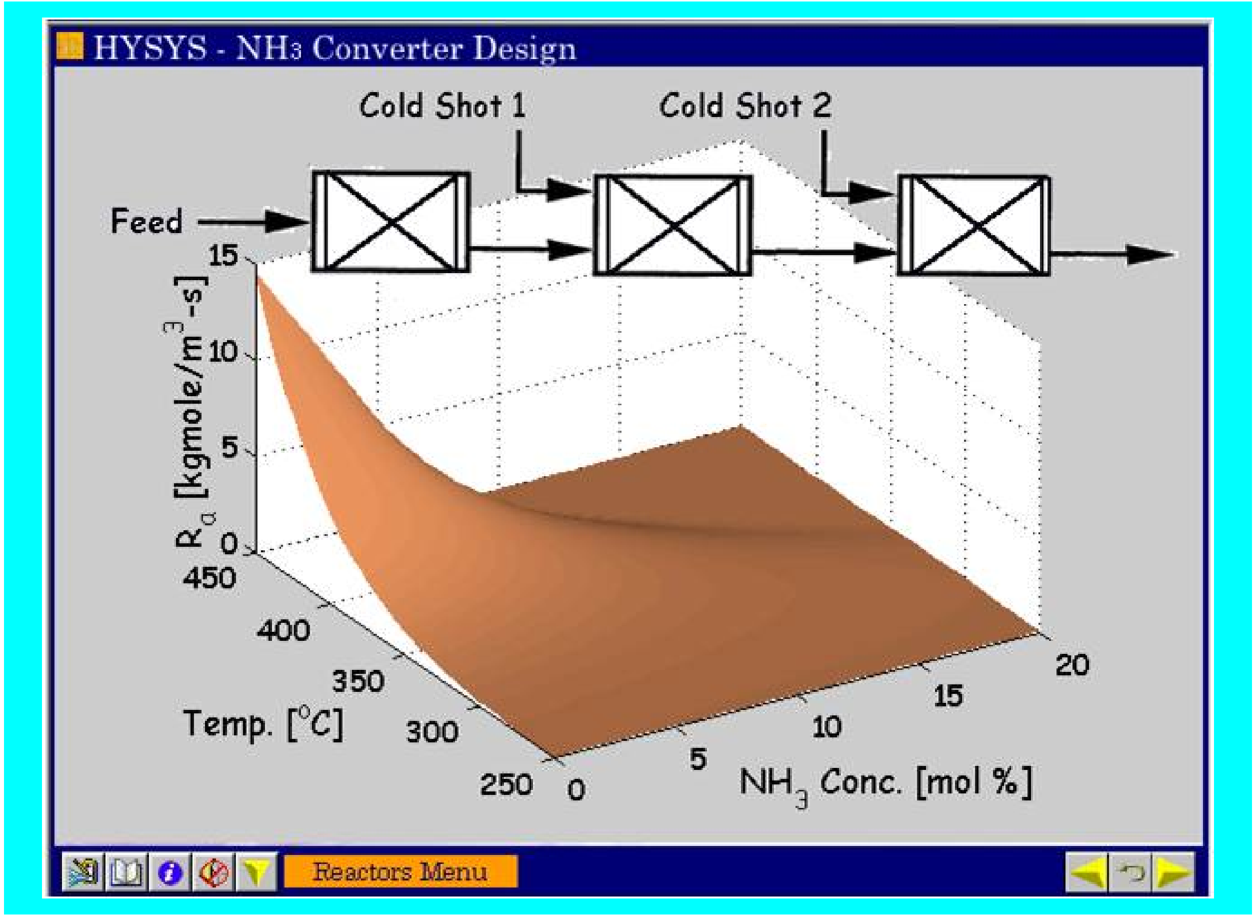
Now suppose 5 lbmole/hr of *dodecane* is added to the reactor feed ($CO : H_2 = 1 : 2$), then, with a complete conversion of CO, the effluent temperature will be reduced to 77.6^oC.



Heat Transfer in Reactors

Heuristics 21

Ex: NH_3 synthesis converter cold-shot optimization



Heat Transfer in Reactors

Heuristics 21

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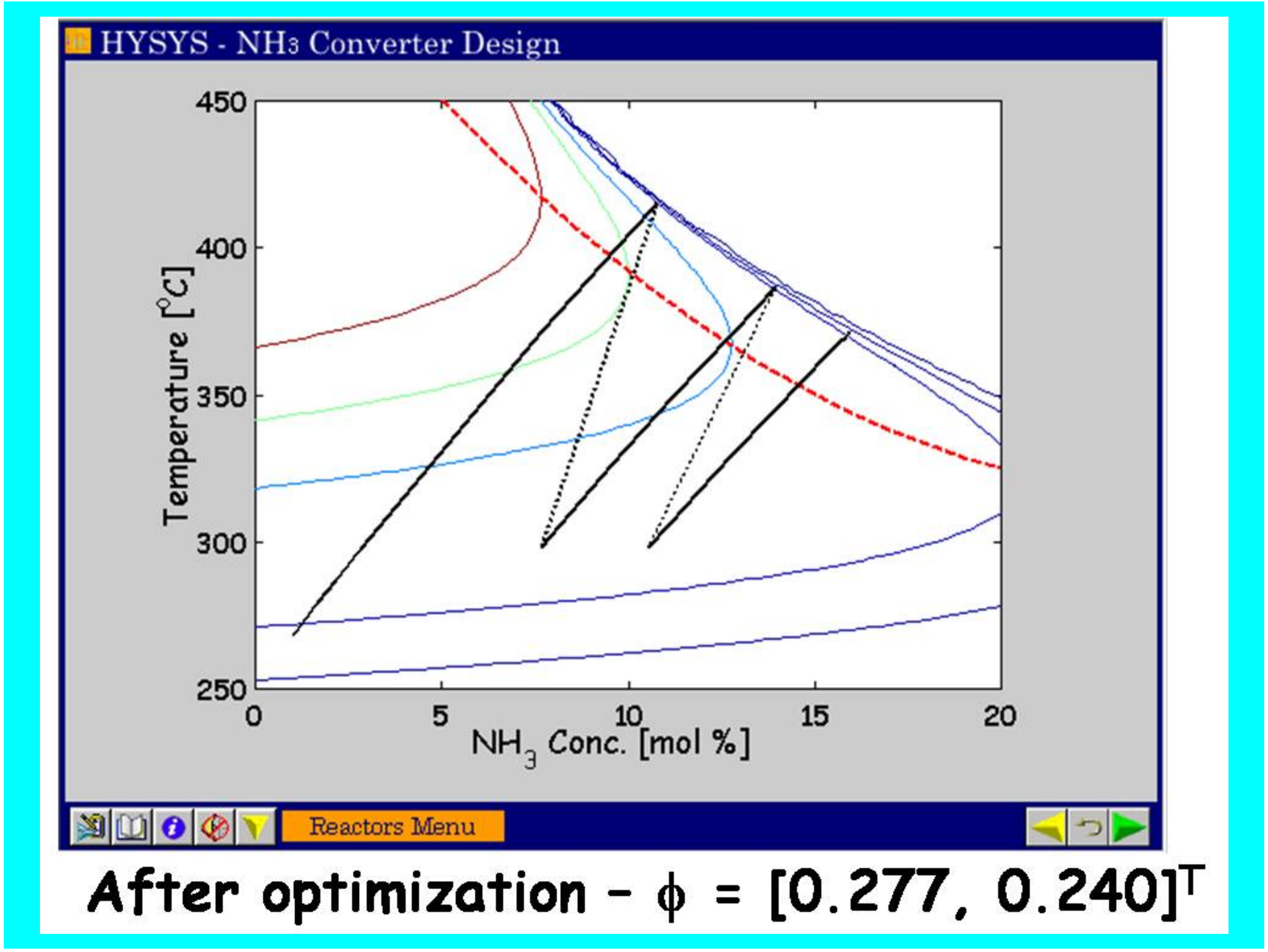
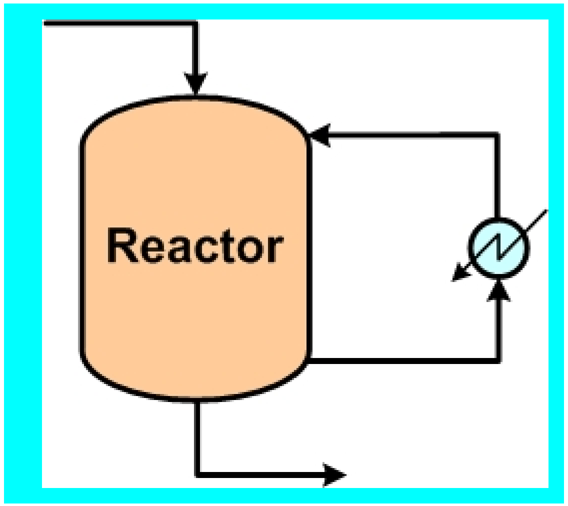


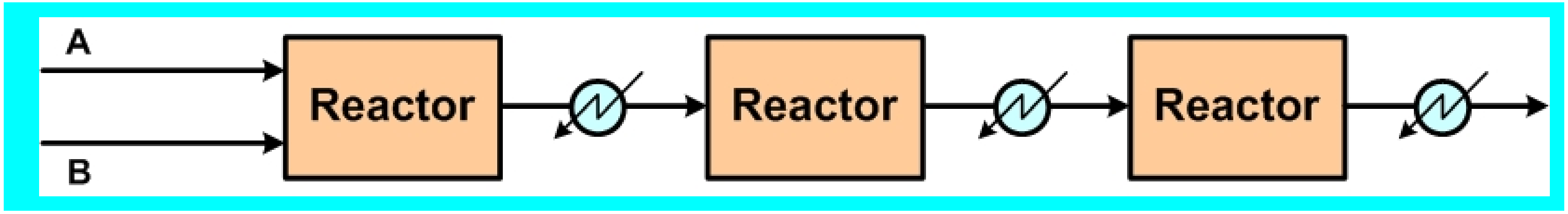
After optimization - $\phi = [0.277, 0.240]^T$

Heat Transfer in Reactors

Heuristics 22

For less exothermic heats of reaction, circulate reactor fluid to an external cooler, or use a jacketed vessel or cooling coils. Also, consider the use of intercoolers.

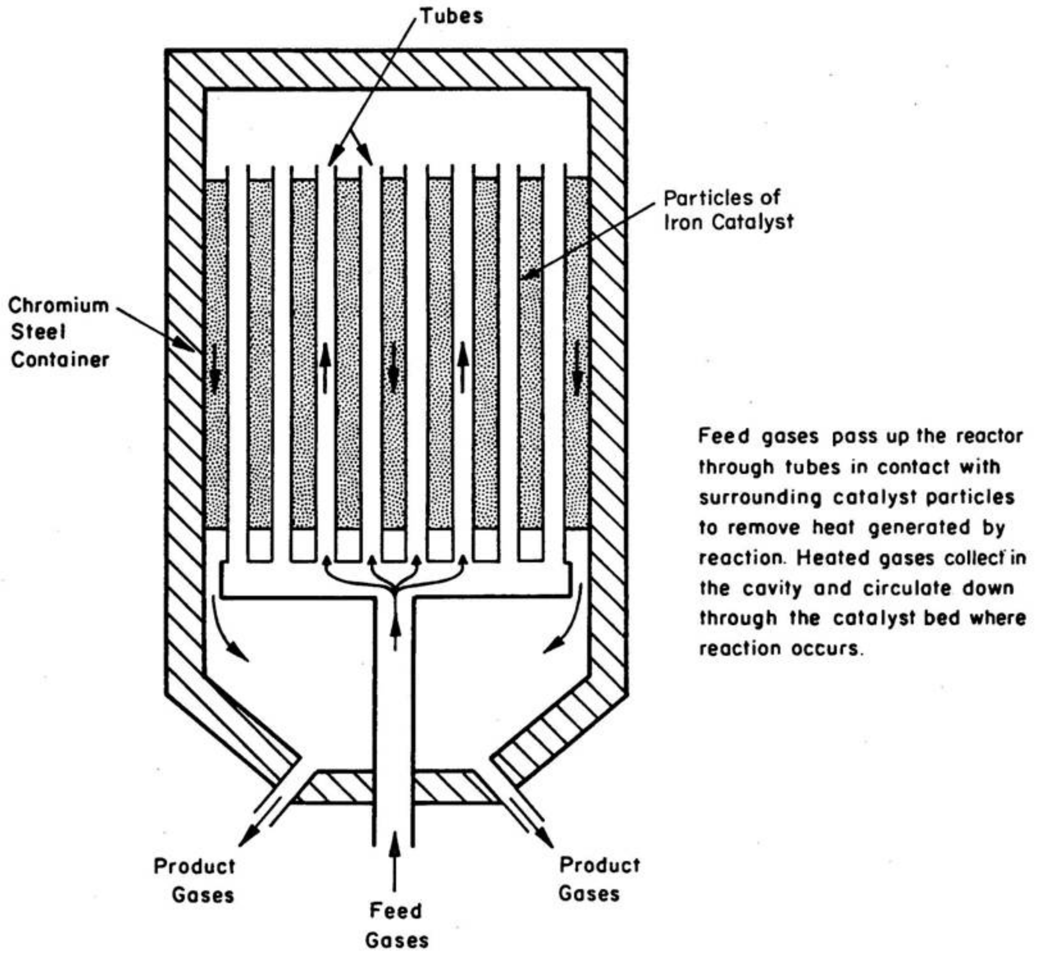




Heat Transfer in Reactors

Heuristics 22

Ex: TVA design for NH_3 synthesis converters



Feed gases pass up the reactor through tubes in contact with surrounding catalyst particles to remove heat generated by reaction. Heated gases collect in the cavity and circulate down through the catalyst bed where reaction occurs.

Heat Transfer in Reactors

Heuristics 23

To control temperature for a highly endothermic heat of reaction, consider the use or excess reactant, an inert diluent, or hot shots. These affect the distribution of chemicals and should be inserted early in process synthesis.

- **Example:**

  When ethylbenzene is pyrolyzed to produce styrene,

  $$\text{Ethylbenzene} \longrightarrow \text{Styrene} + H_2$$

  superheated steam is added to provide the heat of reaction and keep the reaction temperature elevated.

Heat Transfer in Reactors

Heuristics 24

For less endothermic heats of reaction, circulate reactor fluid to an external heater, or use a jacketed vessel or heating coils. Also, consider the use of interheaters between adiabatic reaction stages.

Heat Exchangers and Furnaces

Heuristics 25

Unless required as part of the design of the separator or reactor, provide necessary heat exchange for heating or cooling process fluid streams, with or without utilities, in an external shell-and-tube heat exchanger using countercurrent flow.

However, if a process stream requires healing above 750^oF, use a furnace unless the process liquid is subject to chemical decomposition.

Heat Exchangers and Furnaces

Heuristics 26

Near-optimal minimum temperature approaches in heat exchangers depend on the temperature level as follows:

10^{o}F or less for temperatures below ambient.

20^{o}F for temperatures at or above ambient up to 300^{o}F.

50^{o}F for high temperatures.

250 to 350^{o}F in a furnace for flue gas temperature above inlet process fluid temperature.

Example:

Suppose it is desired to heat $25,000$ lb/hr of toluene at 100^{o}F and 90 psia with $25,000$ lb/hr of styrene at 300^{o}F and 50 psia.

Assume both streams will be liquid, use a shell-and-tube HE with countercurrent flow and a minimum approach temperature of 20^{o}F.

Let the average specific heats of the two streams be 0.43 Btu/lb-^{o}F for toluene and 0.44 Btu/lb-^{o}F for styrene.

Heat Exchangers and Furnaces

Heuristics 26

Example: (continued)

Initially it is not known to which end of the HE the 20^oF minimum approach applies. Assume it applies at the toluene inlet end. If so, the styrene exit temperature is $100+20=120^o$F. This gives a HE duty, based on styrene of:

$$Q = 25,000(0.44)(300-120) = 1,980,000 \text{ Btu/hr}$$

Using this duty, the exit temperature of toluene can be computed.

$$Q = 1,980,000 = 25,000(0.43)(T_{\text{toluene out}} - 100) \text{ Btu/hr}$$

Solving, $T_{\text{toluene out}} = 284.2^o$F. But this gives a temperature approach of $300 - 284.2 = 15.8 < 20^o$F at the styrene inlet end. Therefore, the minimum approach must be applied to the styrene inlet end. Similar calculations give $T_{\text{toluene out}} = 280^o$F and $T_{\text{styrene out}} = 124.1^o$F. This corresponds to an approach temperature at the toluene inlet end of 24.1^oF, which is greater than the minimum approach temperature and, therefore, is acceptable

Heat Exchangers and Furnaces

Heuristics 27

When using cooling water to cool or condense a process stream, assume a water inlet temperature of 90^oF (from a cooling tower) and a maximum water outlet temperature of 120^oF.

Heat Exchangers and Furnaces

Heuristics 28

Boil a pure liquid or close-boiling liquid mixture in a separate heat exchanger, using a maximum overall temperature driving force of 45^oF to ensure nucleate boiling and avoid undesirable film boiling.

When cooling and condensing a gas, both sensible and latent heat can be removed in a single heat exchanger. However, because of many two-phase flow regimes that can occur when boiling a fluid, it is best to provide three separate heat exchangers when changing a subcooled liquid to a superheated gas, especially when the difference between the bubble point and dew point is small. The first exchanger preheats the liquid to the bubble point; the second boils the liquid; the third superheats the vapor.

Heat Exchangers and Furnaces

Heuristics 29

When cooling and condensing a stream in a heat exchanger, a zone analysis should be made to make sure that the temperature difference between the hot stream and the cold stream is equal to or greater than the minimum approach temperature at all locations in the heat exchanger. The zone analysis is performed by dividing the heat exchanger into a number of segments and applying an energy balance to each segment to determine corresponding stream inlet and outlet temperatures for the segment, taking into account any phase change. A process simulation program conveniently accomplishes the zone analysis.

Note: The minimum approach temperature in a countercurrent flow HE may occur at an intermediate location rather than at one of the two ends.

Heat Exchangers and Furnaces

Heuristics 30

Typically, a hydrocarbon gives an adiabatic flame temperature of approximately $3,500^o$F when using the stoichiometric amount of air. However, use excess air to achieve complete combustion and give a maximum flue-gas temperature of $2,000^o$F. Set the stack gas temperature at 650 to 950^oF to prevent condensation of the corrosive components of the flue gas.

Heuristics 31

Estimate heat-exchanger pressure drops as follows:

1.5 psi for boiling and condensing.
3 psi for a gas.
5 psi for a low-viscosity liquid.
7-9 psi for a high-viscosity liquid.
20 psi for a process fluid passing through a furnace.

Heat Exchangers and Furnaces

Heuristics 32

Quench a very hot process stream to at least $1,150^o$F before sending it to a heat exchanger for additional cooling and/or condensation. The quench fluid is best obtained from a downstream separator. Alternatively, if the process stream contains water vapor, liquid water may be an effective quench fluid.

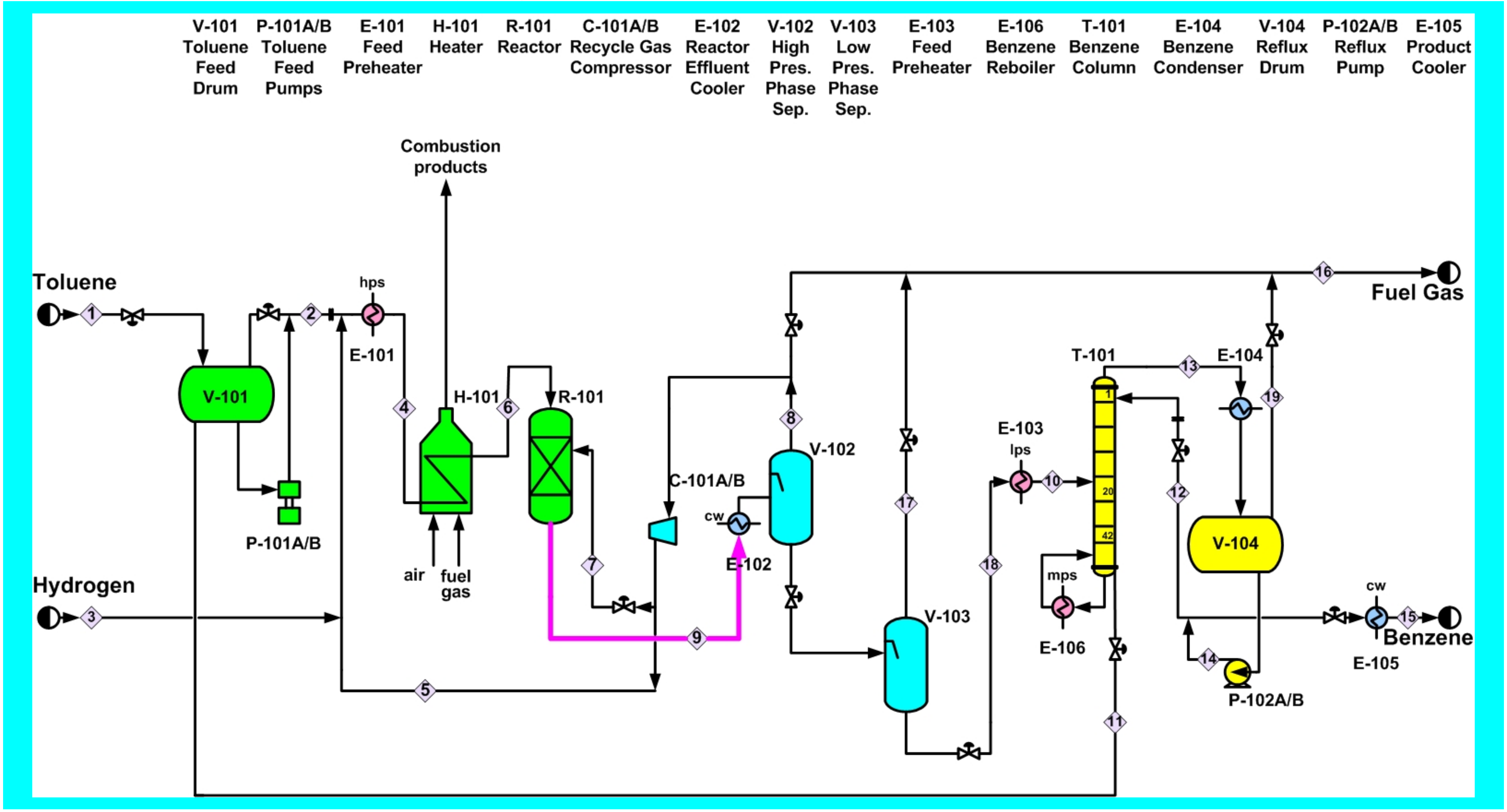
Note: Unless exotic materials are used, HEs should not be used for cooling and/or condensing process streams with temperatures above $1,150^o$F.

Heat Exchangers and Furnaces

Heuristics 32

EX: Toluene HDA process

$$C_7H_8 + H_2 \longrightarrow C_6H_6 + CH_4$$

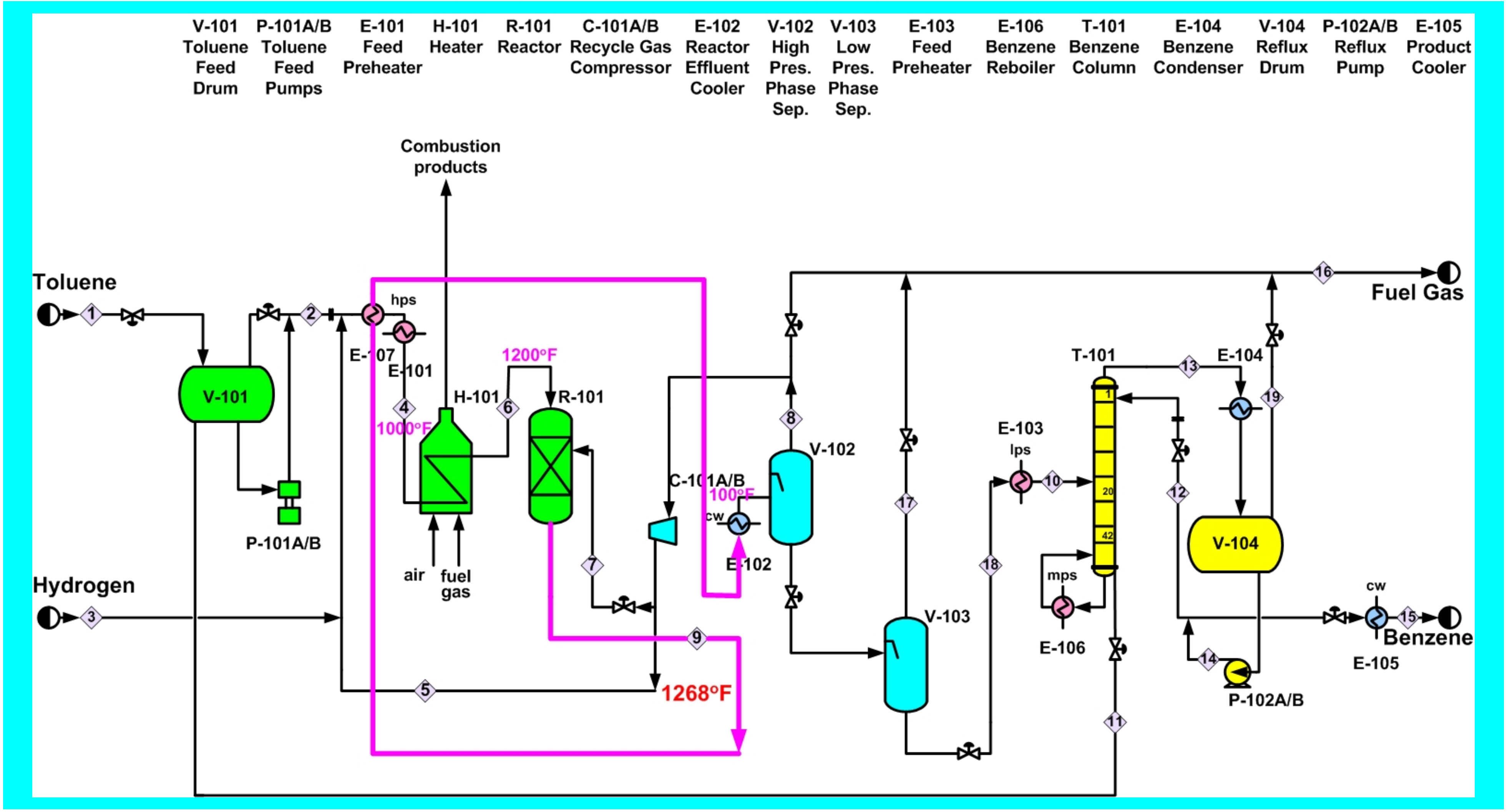


Heat Exchangers and Furnaces

Heuristics 32

EX: Toluene HDA process — heat recovery

$$C_7H_8 + H_2 \longrightarrow C_6H_6 + CH_4$$

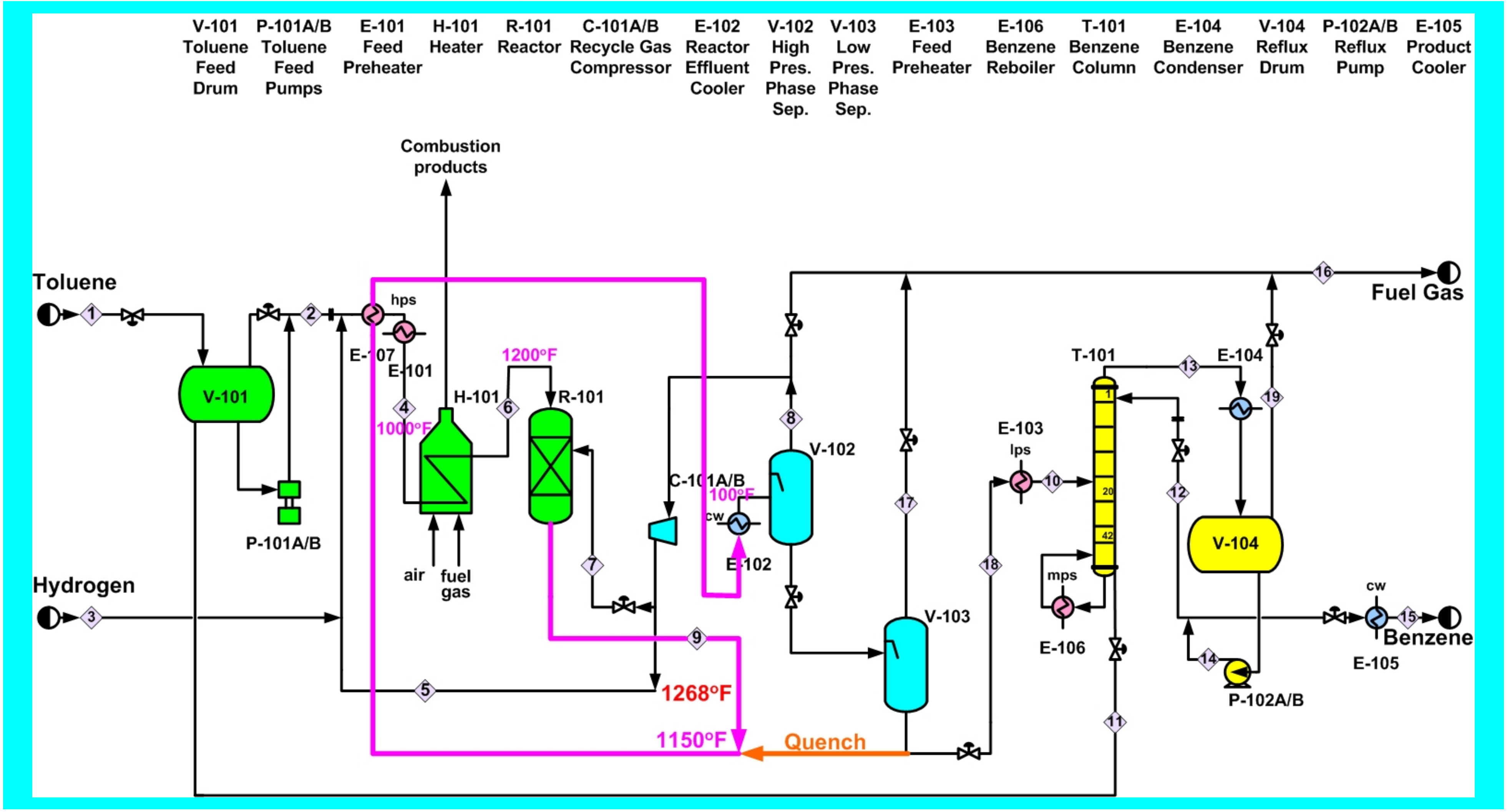


Heat Exchangers and Furnaces

Heuristics 32

EX: Quench stream from downstream separator

$$C_7H_8 + H_2 \longrightarrow C_6H_6 + CH_4$$



Heat Exchangers and Furnaces

Heuristics 33

If possible, heat or cool a stream of solid particles by direct contact with a hot gas or cold gas, respectively, using a rotary kiln, a fluidized bed, a multiple hearth, or a flash/pneumatic conveyor. Otherwise, use a jacketed spiral conveyor.

Note: Streams of solid particles are commonly heated or cooled directly or indirectly. Heat transfer is much more rapid and controllable when using direct heat exchange.

Pressure Increase Operations

Heuristics 34

Use a fan to raise the gas pressure from atmospheric pressure to as high as 40 inches water gauge (10.1 kPa gauge or 1.47 psig).

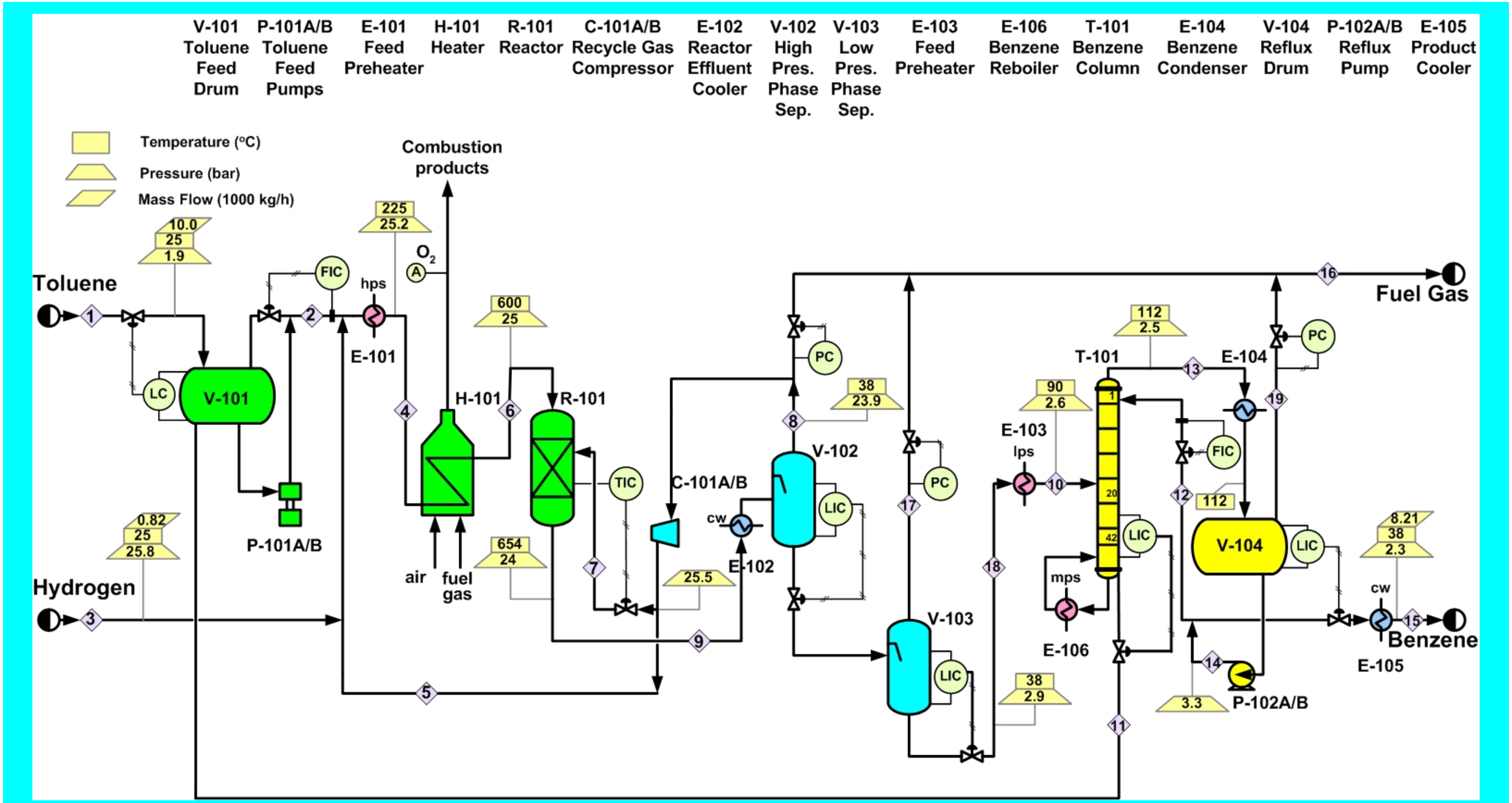
Use a blower or compressor to raise the gas pressure to as high as 206 kPa gauge or 30 psig.

Use a compressor or a staged compressor system to attain pressures greater than 206 kPa gauge or 30 psig.

Pressure Increase Operations

Heuristics 34

For the toluene hydrodealkylation process, the pressure of the recycle gas leaving the flash drum at 100^oF and 484 psia is increased with a compressor to 569 psia, so that, after pressure drops of 5 psia through the HE and 70 psia through the furnace, it enters the reactor at a required pressure of 494 psia.



Pressure Increase Operations

Heuristics 35

Estimate the theoretical adiabatic horsepower (THp) for compressing a gas from:

$$\text{THp} = \text{SCFM}\left(\frac{T_1}{8,130a}\right)\left[\left(\frac{P_2}{P_1}\right)^a - 1\right]$$

where SCFM $=$ standard cubic feet of gas per minute at 60^oF and 1 atm (379 SCF/lbrmol), T_1 $=$ gas inlet temperature in ^{o}R, inlet and outlet pressures, P_1 and P_2, are absolute pressures, and $a = (k-1)/k$, with k $=$ the gas specific heat ratio, C_p/C_v.

Estimate the theoretical exit temperature, T_2 for a gas compressor from:

$$T_2 = T_1\left(\frac{P_2}{P_1}\right)^a$$

Pressure Increase Operations

Heuristics 35

Example:

If air at 100^oF is compressed from 1 to 3 atm (compression ratio $= 3$), usin $k = 1.4$, the THp is computed to be 128 Hp/standard million ft^3/day, with an outlet temperature $= 306^o$F.

When using a compressor, the gas theoretical exit temperature should not exceed approximately 375^oF. This corresponds to a compression ratio of 4 for $k = 1.4$ and $T_2 = 375^o$F.

$\Rightarrow$ multistage compression with intercoolers.

Pressure Increase Operations

Heuristics 36

Estimate the number of gas compression stages, N, from the following table, which assumes a specific heat ratio of 1.4 and a maximum compression ratio of 4 for each stage.

Final Pessure/Inlet Pressure	Number of Stages
< 4	1
4 to 16	2
16 to 64	3
64 to 256	4

Optimal interstage pressures correspond to equal Hp for each compressor. Therefore, based on the above equation for theoretical compressor Hp, estimate interstage pressures by using approximately the same compression ratio for each stage with an intercooler pressure drop of 2 psi or 15 kPa.

Pressure Increase Operations

Heuristics 36

Example:

A feed gas at 100^oF and 30 psia is to be compressed to 569 psia. With an overall compression ratio of $569/30 = 19$, a 3-stage system is indicated. For equal compression ratios, the compression ratio for each stage of a 3-stage system $= 19^{1/3} = 2.7$. The estimated stage pressures are as follows, taking into account a 2 psi drop for each intercooler and its associated piping:

Stage	Compressor Inlet P, psia	Compressor Outlet P, psia
1	30	81
2	79	213
3	211	569

Pressure Increase Operations

Heuristics 37

For heads up $103,200$ ft and flow rates in the range of to to $5,000$ gpm, use a centrifugal pump.

For high heads up to $20,000$ ft and flow rates up to 500 gpm, use a reciprocating pump.

Less common are axial pumps for heads up to 40 ft for flow rates in the range of 20 to $100,000$ gpm and rotary pumps for heads up to $3,000$ ft for flow rates in the range of 1 to $1,500$ gpm.

Note: The head in feet is the pressure increase across the pump in pounds force/ft^2 divided by the liquid density in lb/ft^3.

For liquid water, with a density of 62.4 lb/ft^3, heads of $3,000$ and $20,000$ ft correspond to pressure increases across the pump of $1,300$ and $8,680$ psi, respectively.

Pressure Increase Operations

Heuristics 38

For liquid flow, assume a pipeline pressure drop of 2 psi/100 ft of pipe and a control valve pressure drop of at least 10 psi.
For each 10-ft rise in elevation, assume a pressure drop of 4 psi.

Heuristics 39

Estimate the theoretical horsepower (THp) for pumping a liquid from:

$$\text{THp} = \frac{\text{(gpm)(Pressure increase, psi)}}{1,714}$$

Heuristics 40

Consider the use of an expander for reducing the pressure of a gas or a pressure recovery turbine for reducing the pressure of a liquid when more than 20 Hp and 150 Hp, respectively, can be recovered.

Pressure Decrease Operations

Heuristics 41

Estimate the theoretical adiabatic horsepower (THp) for expanding a gas from:

$$\text{THp} = \text{SCFM}\left(\frac{T_1}{8,130a}\right)\left[1 - \left(\frac{P_2}{P_1}\right)^a\right]$$

Heuristics 42

Estimate the theoretical horsepower (THp) for reducing the pressure of a liquid from:

$$\text{THp} = \frac{(\text{gpm})(\text{Pressure decrease, psi})}{1,714}$$

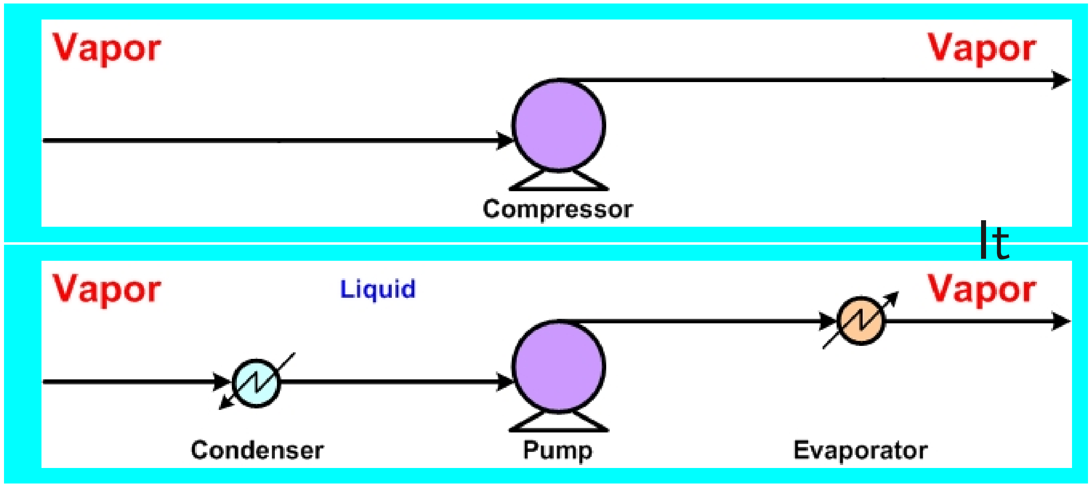
Pumping and Compression

Heuristics 43

To increase the pressure of a stream, pump a liquid rather than compress a gas; that is, condense a vapor, as long as refrigeration (and compression) is not needed, before pumping.

Since work done by pumping or compressions is given by:

$$W = \int_{V_1}^{V_2} V\,dP$$



It follows that it is more efficient to pump a liquid than to compress a gas. Thus, it is almost always preferable to condense a vapor, pump it, and vaporize it, rather than compress it.

Exception: if condensation requiresrefrigeration.

Pumping and Compression

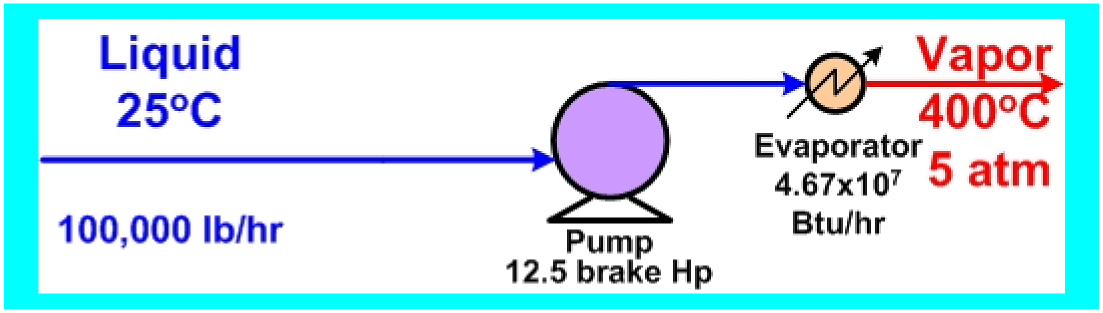
Heuristics 43

Example: Feed Preparation of Ethylbenzene

Ethylbenzene is to be taken from storage at 25^oC and 1 atm and fed to a styrene reactor at 400^oC and 5 atm at $100,000$ lb/h.

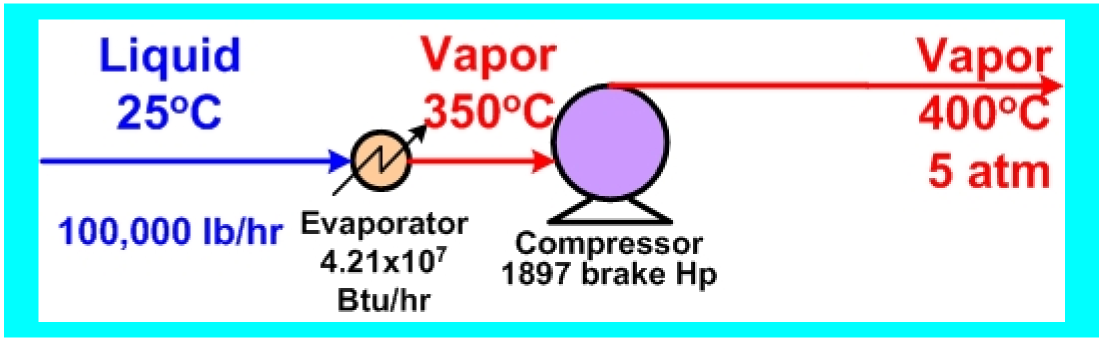
Alternative 1: Pump the liquid first.

12.5 brake Hp to pump, 4.67×10^7 Btu/hr to vaporize



Alternative 2: Vaporize the liquid first.

4.21×10^7 Btu/hr to vaporize, 1897 brake Hp to compress



Vacuum

- When process pressures less than the ambient pressure are required (common in crystallization, distillation, drying, evaporation, pervaporation), vacuum devices are needed.
- A vacuum system is used to remove the air together with any associated vapor in the process stream that pass through the equipment.
  A vacuum inside equipment causes inleakage of ambient-pressure air
- For continuous operation, vacuums are predominantly in the range of 1 to 760 torr (0.13 to 101.3 kPa).
- It is common to use a vacuum pump, which compresses the gas from vacuum (suction pressure) to ambient pressure;
  or a jet-ejector system, which uses a flow of pressurized water or steam to mix with and remove the gas to create the vacuum.
- To design the vacuum system, it is necessary to estimate the inleakage of air, determine the total amount of gas (inleakage plus associated vapor) to be removed, and select an appropriate system for the vacuum level required.

Vacuum

Heuristics 44

Estimate inleakage of air by:

$$w = kV^{0.667}$$

where $w =$ lb/hr of air inleakage,
$V =$ ft^3 of volume of the equipment under vacuum, and
$k = 0.20$ for pressures greater than 90 torr,
$k = 0.15$ for pressures between 21 and 89 torr,
$k = 0.10$ for pressures between 3 and 20 torr, and
$k = .051$ for pressures between 1 and 3 torr.

Vacuum

Heuristics 45

To reduce the amount of gas sent to the vacuum system if its temperature is greater than 100^oF, add a condenser using cooling water before the vacuum system. The gas leaving the condenser will be at a dew-point temperature of 100^oF at the vacuum pressure.

Heuristics 46

For pressures down to 10 torr and gas flow rates up to $10,000$ ft^3/min at the inlet to the vacuum system, use a liquid-ring vacuum pump.

For pressures down to 2 torr and gas flow rates up to $1,000,000$ ft^3/min at the inlet to the vacuum system, use a steam-jet ejeclor system (one-stage for 100 to 760 torr, two-stage for 15 to 100 torr, and three-stage for 2 to 15 torr). Include a direct-contact condenser between stages.

Vacuum

Heuristics 47

For a three-stage steam-jet ejector system used to achieve a vacuum of 2 torr, 100 pounds of 100 psig steam per pound of gas are required.

Heuristics 48

If the solid particles are small in size, low in particle density, and are not sticky or abrasive, use pneumatic conveying with air at 1 to 7 ft^3/ft^3 of solids and 35 to 120 ft/s air velocity for distances up to 400 ft.
Otherwise, for sticky and/or abrasive solids of any size and density, use a screw conveyer and/or bucket elevator for distances up to 150 ft.
For solid particles of any size and shape, and not sticky, use a belt conveyor, with inclination up to 30^o if necessary, for long distances up to a mile or more.

Solid Particle Size Change and Separation

- It is frequently necessary to change the particle size of solids to meet product specifications or change reaction or drying rate.
- Methods to accomplish changes in particle size include:
  - crushing, grinding, and disintegration to reduce particle size;
  - compression, extrusion, and agglomeration to increase particle size;
  - and size separation devices to obtain a narrow range of particle size.
- Crushers and grinders are used with screens in closed circuits, where oversize material is recycled.
- Grindability is determined mainly by hardness as measured by the following Mohs scale, which ranges from 1 for the softest material to 10 for the hardest:

Solid Particle Size Change and Separation

Material	**Mohs Scale**
Talc, $Mg_3SiO_{10}(OH)_2$	1
Gypsum, $CaSO_4 \cdot 2H_2O$	2
Calcite, $CaCO_3$	3
Fluorite, CaF_2	4
Apatite, $Ca_5(PO_4)_3(OH, F, Cl)$	5
Feldspar, Na, Ca, K, Al silicates	6
Quartz, SiO_2	7
Topaz, $Al_2SiO_4(F, OH)_3$	8
Corundum, Al_2O_3	9
Diamond, C	10

- Materials with a Mohs scale from 1 to 3 are considered soft and include graphite, many plastics, asphalt, sulfur, many inorganic salts, marble, and anthracite coal.
- Intermediate hardness extends from Mohs scale of 4 to 6 and includes limestone, asbestos, and glass.
- Hard materials are characterized by a Mohs scale of 7 to 10 and include sand, granite, and emery.

Solid Particle Size Change and Separation

- Size of small particles is commonly stated in terms of screen mesh size according to the following U.S. standard (ASTM EII), where not all mesh sizes are given:

Mesh (Openings/inch)	Sieve Opening, mm
4	4.75
6	3.35
8	2.36
12	1.70
16	1.18
20	0.841
30	0.600
40	0.420
50	0.300
70	0.212
100	0.149
140	0.106
200	0.074
270	0.053
400	0.037

- The following heuristics apply to particle-size reduction.

Solid Particle Size Change and Separation

Heuristics 49

Crushing of coarse solids. Use a jaw crusher to reduce lumps of hard, abrasive, and/or sticky materials of 4 inches to 3 feet in diameter to slabby particles of 1 to 4 inches in size.

Use a gyratory clusher to reduce slab by materials of 8 inches to 6 feet in size to rounded particles of 1 to 10 inches in diameter.

Use a cone crusher to reduce less hard and less sticky materials of 2 inches to 1 foot in diameter to particles of 0.2 inch (4 mesh) to 2 inches in diameter.

Solid Particle Size Change and Separation

Heuristics 50

Gringing to fine solids. Use a rod mill to take particles of intermediate hardness as large as 20 mm and reduce them to pal1icles in the range of 10 to 35 mesh.

Use a ball mill to reduce particles of low to intermediale hardness of 1 to 10 mm in size to very small particles of less than 140 mesh.

Solid Particle Size Change and Separation

Heuristics 51

Particle-size enlargement. Use compression with rotary compression machines to convert powders and granules into tablets of up to 1.5 inches in diameter.

Use extruders with cutters to make pellets and wafers from pastes and melts.

Use roll compactors to produce sheets from finely divided materials; the sheets are then cut into any desired shape.

Use rotating drum granulators and rotary disk granulators with binders to produce particles in the size range of 2 to 25 mm.

Solid Particle Size Change and Separation

Heuristics 52

Size separation of particles. Use a grizzly of spaced, inclined, vibrated parallel bars to remove large particles greater than 2 inches in diameter.

Use a revolving cylindriical perforated screen to remove intermediate-size particles in the size range of 0.25 inch to 1.5 inches in diameter.

Use flat, inclined woven screens (U.S. standard) that are vibrated, shaken, or impacted with bouncing balls to separate small particles in the size range of 3 to 80 mesh.

Use an air classifier to separate fine particles smaller than 80 mesh.

Removal of Particle from Gases and Liquids

Heuristics 53

Use a cyclone separator to remove, from a gas, droplets or solid particles of diameter down to 10 microns (0.01 mm).

Use a hydroclone separator to remove, from a liquid, insoluble liquid droplets or solid particles of diameter down to 5 microns (0.005 mm).

However, small amounts of entrained liquid droplets are commonly removed from gases by vertical knock-out drum equipped with mesh pads to help coalesce the smallest droplets

- Fine particles are most efficiently removed from dilute suspensions in gases and liquids by using centrifugal force in cyclones and hydroclones, respectively.

Heuristics for Process Synthesis: Summary

We have focused some design heuristics, enabling you to:

- Understand the importance of selecting reaction paths that do not involve toxic or hazardous chemicals, or to reduce their presence by shortening residence times in the process units and avoiding their storage in large quantities.
- Be able to distribute the chemicals in a process flowsheet, to account for the presence of inert species, to purge species that would otherwise build up to unacceptable concentrations, to achieve a high selectivity to the desired products.
- Be able to apply heuristics in selecting separation processes to separate liquids, vapors, and vapor-liquid mixtures.
- Be able to distribute the chemicals to remove exothermic heats of reaction.
- Understand the advantages of pumping a liquid rather than compressing a vapor.

Thank You for Your Attention

Questions Are Welcome