Chapter 4
Lecture # 2-2

- **Conditions of Special Concern for the Operation of Some Equipment .**

- **Analysis of Important Process Conditions**

Conditions of Special Concern

Table 4.4 Changes in Process Conditions That Are of Special Concern for a Stream Passing through a Single Piece of Equipment

Type of Equipment	Change in Stream Condition Causing Concern	Justification or Remedy	Penalty for Operating Equipment in this Manner
1. Compressors	$P_{out}/P_{in} > 3$	**Remedy:** Use multiple stages and intercoolers	High theoretical work requirement due to large temperature rise of gas stream
	High temperature inlet gas	**Remedy:** Cool the gas before compression.	High theoretical work requirement and special construction materials required
2. Heat Exchangers	$\Delta T_{lm} > 100°C$	**Remedy:** Integrate heat better within process (see Chapter 13)	Large temperature driving force means we are wasting valuable high-temperature energy
		Justification: Heat integration not possible or not profitable	

Conditions of Special Concern

3. Process Heaters	$T_{out} < T_{steam\ available}$	**Remedy:** Use high-pressure steam to heat process stream **Justification:** Heater may be needed during start-up	Process heaters are expensive and unnecessary if heating may be accomplished by using an available utility
4. Valves	Large ΔP across valve	**Remedy:** For gas streams install a turbine to recover lost work **Justification:** (a) Valve used for control purposes (b) Installation of turbine not profitable (c) Liquid is being throttled	Wasteful expenditure of energy due to throttling

Conditions of Special Concern

5. Mixers (streams mixing)	Streams of greatly differing temperatures mix	**Remedy:** Bring temperatures of streams closer together using heat integration	Wasteful expenditure of high-temperature energy
	Streams of greatly differing composition mix	**Justification:** (a) Quenching of reaction products (b) Provides driving force for mass transfer	Causes extra separation equipment and cost

Conditions of Special Concern

Example 4.2

It is necessary to provide a nitrogen stream at 80°C and a pressure of 6 bar. The source of the nitrogen is at 200°C and 1.2 bar. Determine the work and cooling duty required for three alternatives.

- **a.** Compress in a single compression stage and cool the compressed gas.
- **b.** Cool the feed gas to 80°C and then repeat Part a, above.
- **c.** Repeat Part b, above, except use two stages of compression with an intercooler.
- **d.** Identify any conditions of special concern that occur.

Nitrogen can be treated as an ideal diatomic gas for this comparison. Use as a basis 1 kmol of nitrogen and assume that the efficiency, ε, of each stage of compression is 70%.

For ideal diatomic gas: $C_p = 3.5R$, $C_v = 2.5R$, $\gamma = C_p/C_v = 1.4$, $R = 8.314$ kJ/kmol K, $\varepsilon = 0.70$

Equations used: $q = C_p\Delta T$, $w = RT_{in}\gamma/(\gamma-1)[(P_{out}/P_{in})^{(\gamma-1)/\gamma} - 1]/\varepsilon$,

$$T_{out} = T_{in}(1 + 1/\varepsilon)[(P_{out}/P_{in})^{(\gamma-1)/\gamma} - 1]$$

Conditions of Special Concern

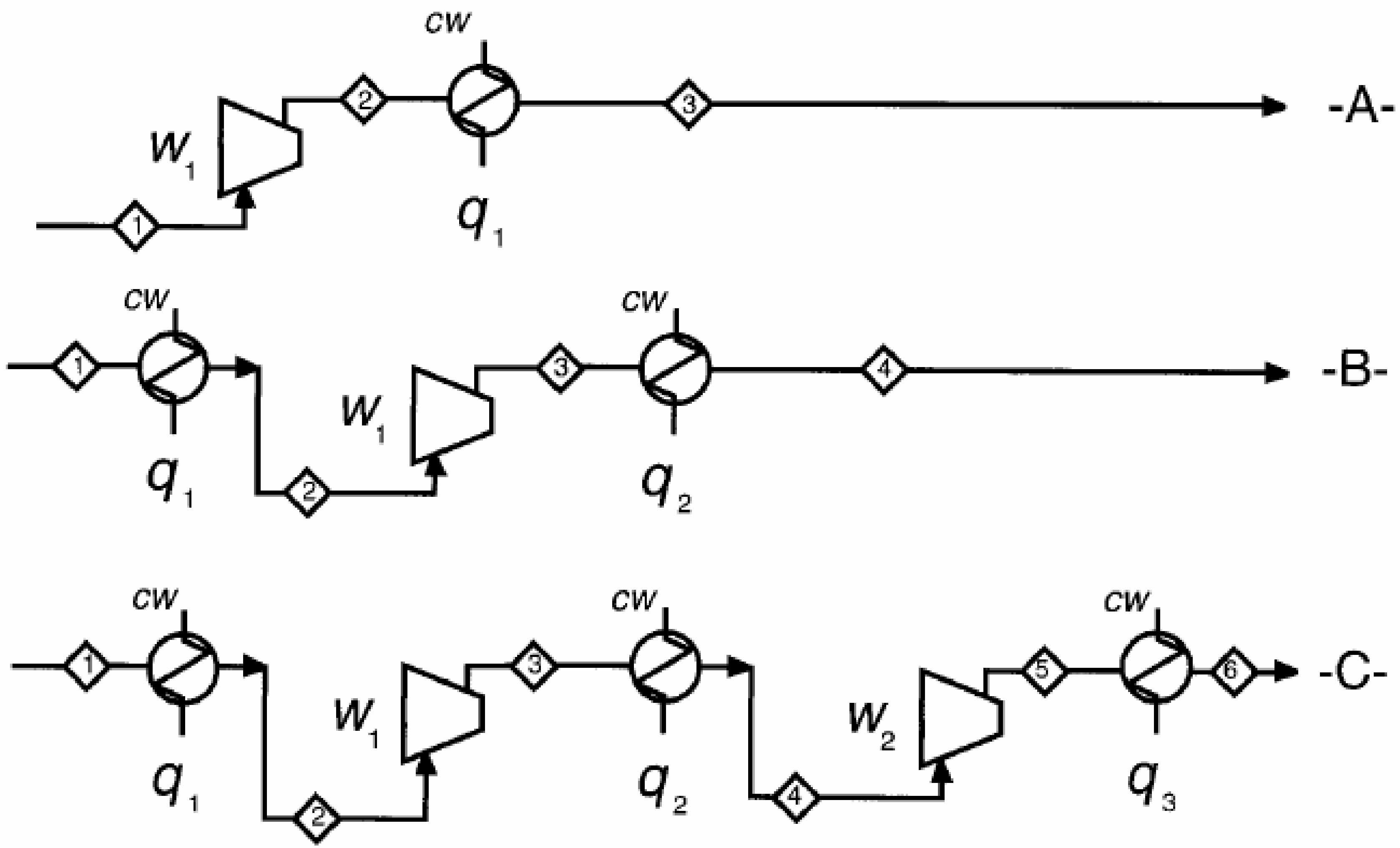


Figure E4.2 Alternative Process Schemes for Compression of Nitrogen

Conditions of Special Concern

Table E4.2 Flow Summary Table for Example 4.2 and Figure E4.2

Stream No. in Figure E4.2	System -A- T(°C)	System -A- P(bar)	System -B- T(°C)	System -B- P(bar)	System -C- T(°C)	System -C- P(bar)
1	200	1.2	200	1.2	200	1.2
2	595	6.0	80	1.2	80	1.2
3	80	6.0	374	6.0	210	2.68
4	—	—	80	6.0	80	2.68
5	—	—	—	—	210	6.0
6	—	—	—	—	80	6.0
Work: kJ/kmol						
w_1	11,470		8560		3780	
w_2	—		—		3780	
w_{total}	11,470		8560		7560	
Heat: kJ/kmol						
q_1	14,970		3490		3490	
q_2	—		8550		3780	
q_3	—		—		3780	
q_{total}	14,970		12,040		11,050	

Conditions of Special Concern

Figure E4.2 gives the process flow diagrams for the three alternatives and identifies stream numbers and utilities.

The results of the calculations for Parts a, b, and c are provided in Table E4.2, which shows stream conditions and utility requirements. To keep the calculations simple, the pressure drops across and between equipment have been ignored.

Part d: Alternative -A- requires a compressor exit temperature of 595°C that is a condition of special concern. Note also that although the intermediate temperature of the gas (stream) in Alternative -B- was 374°C, because this stream is to be cooled there are no concerns about utility requirements.

Analysis of Important Process Conditions

Table 4.5 Process Conditions Matrix for the PFD of the Toluene Hydrodealkylation Process Shown in Figure 1.5

	Reactors and Separators Tables 4.1–4.3					Other Equipment Table 4.4				
Equipment	*High Temp*	*Low Temp*	*High Pres.*	*Low Pres.*	*Non-Stoich. Feed*	*Comp*	*Exch.*	*Htr.*	*Valve*	*Mix*
R-101	X		X		X					
V-101										
V-102			X							
V-103										
V-104										
T-101										
H-101										
E-101							X			
E-102							X			

Analysis of Important Process Conditions

Table 4.5 Process Conditions Matrix for the PFD of the Toluene Hydrodealklyation Process Shown in Figure 1.5

	Reactors and Separators Tables 4.1–4.3					Other Equipment Table 4.4				
Equipment	*High Temp*	*Low Temp*	*High Pres.*	*Low Pres.*	*Non-Stoich. Feed*	*Comp*	*Exch.*	*Htr.*	*Valve*	*Mix*
E-103										
E-104										
E-105										
E-106										
C-101										
P-101										
P-102										
PCV on Stream 8									X	
PCV on Stream from V-101 to V-103									X	

Analysis of Important Process Conditions

Evaluation of Reactor R-101

- Three conditions of concern
  - High Temperature
  - High Pressure
  - Non-stoichiometric Feed Conditions

Analysis of Important Process Conditions

Additional Information about toluene HDA reaction

Table 4.6 Equilibrium and Reaction Kinetics Data for the Toluene Hydrodealkylation Process

Reaction Stoichiometry

$$\underset{\text{toluene}}{C_6H_5CH_3} + H_2 = \underset{\text{benzene}}{C_6H_6} + CH_4$$

Equilibrium Constant (*T* is in units of K)

$$\ln(K_p) = 13.51 + \frac{5037}{T} - 2.073\ln(T) + 3.499 \times 10^{-4}T + 4.173 \times 10^{-8}T^2 + \frac{3017}{T^2}$$

Heat of Reaction

$$\Delta H_{reaction} = -37{,}190 - 17.24T + 29.09 \times 10^{-4}T^2 + 0.6939 \times 10^{-6}T^3 + \frac{50{,}160}{T} \quad \frac{\text{kJ}}{\text{kmol}}$$

At the Reaction Conditions of 600°C (873 K)

Equilibrium Constant, $K_p = 265$

Heat of Reaction, $\Delta H_{reaction} = -49{,}500 \quad \frac{\text{kJ}}{\text{kmol}}$

Information on Reaction Kinetics

No side reactions

Reaction is kinetically controlled

Analysis of Important Process Conditions

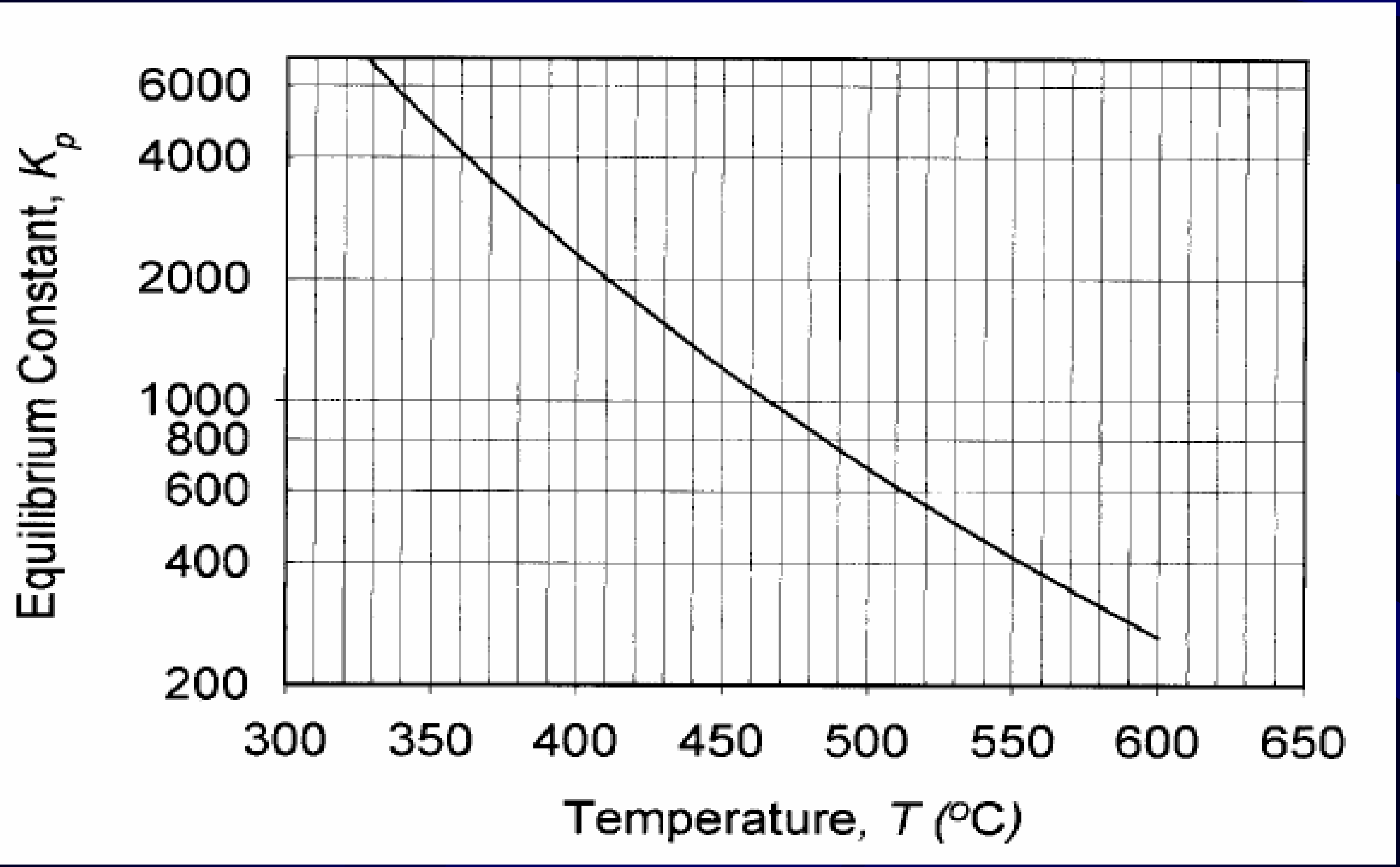
Reactor Analysis

The analysis of the reactor takes place in two parts.

a. Evaluation of the special conditions from the thermodynamic point of view. This assumes that chemical equilibrium is reached and provides a limiting case.

b. Evaluation of the special conditions from the kinetics point of view. This accounts for the limitations imposed by reaction kinetics, mass transfer, and heat transfer.

Analysis of Important Process Conditions



Analysis of Important Process Conditions

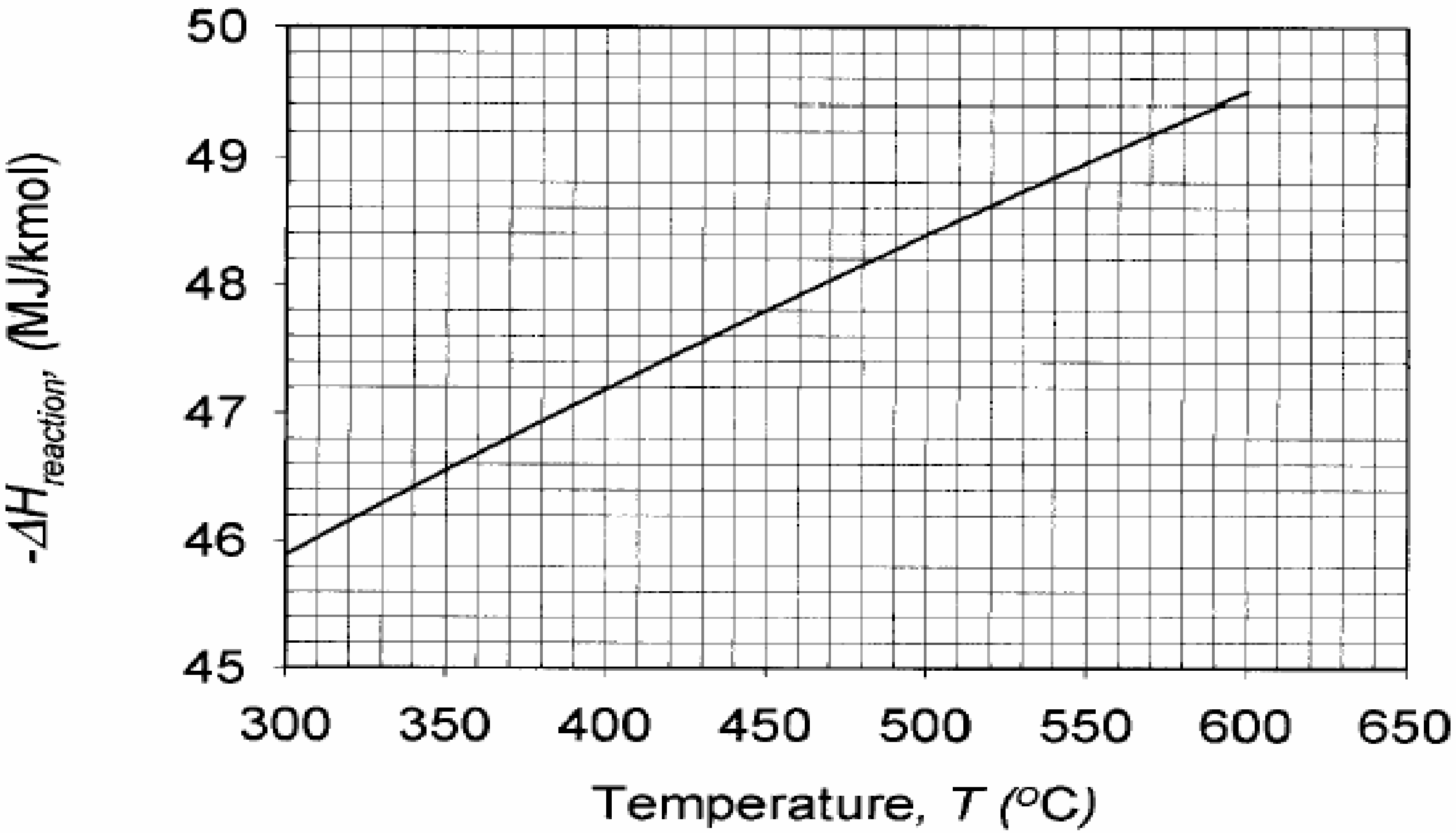


Figure 4.1 Equilibrium Constant and Heat of Reaction as a Function of Temperature for the Toluene Hydrodealkylation Reaction

Analysis of Important Process Conditions

Thermodynamic Consideration

- High temperature concern
  - Fig 4.1 implies the rxn is exothermic
  - For exothermic rxn, as T↑, Xeq↓
  - Decrease in Xeq is undesirable
  - Use of high T cannot be justified from thermodynamic point of view

Analysis of Important Process Conditions

Thermodynamic Consideration

- High pressure concern
  - Rxn stoichiometry shows that there are equal number of reactant and product moles in the HDA rxn.
  - Thus, no effect of pressure on Xeq
  - No reason to use high P from thermodynamic point of view

Analysis of Important Process Conditions

Example 4.3

For the PFD presented in Figure 1.5:

a. Calculate the actual conversion

b. Evaluate the equilibrium conversion at 600°C.

Assuming ideal gas behavior: $K_p = (N_{benzene} N_{methane})/(N_{toluene} N_{hydrogen})$
where N represents the moles of each species at equilibrium

Information on the feed stream to the reactor from Table 1.5 (Stream 6 on Figure 1.5).

Hydrogen	735.4 kmol/h
Methane	317.3
Benzene	7.6
Toluene	144.0
Total	1204.3

Analysis of Important Process Conditions

a. Actual Conversion: Toluene in exit stream (Stream 9) = 36 kmol/h

Conversion = (144 – 36)/144 = 0.75 (75%)

b. Equilibrium Conversion at 600°C. From Table 8.6 @600°C K_y = 265

Let N = kmol/h of benzene formed

$265 = [(N + 7.6)(N + 317.3)]/[(735.4 - N)(144 - N)]$

$N = 143.5$

Equilibrium Conversion = 143.6/144 = 0.997 (99.7%)

Analysis of Important Process Conditions

Example 4.4

(Reference Example 4.3) Reduce the amount of hydrogen in the feed to the reactor to the stoichiometric amount, that is, 144 kmol/h, and determine the effect on the equilibrium conversion at 600°C.

The calculations are not shown. They are similar to those in Example 4.3(b). The total moles of hydrogen in the feed were changed from 790.6 kmol/h to the stoichiometric value of 144 kmol/h.

The results obtained were N = 128.8 kmol/h, Equilibrium Conversion = 0.894 (89.4%).

Conclusions

- T < 40ºC – Refrigeration
- T > 250ºC – Fired Heater or Furnace
- T > 400ºC – M.O.C. Issues
- P < 1 atm – Vacuum and Large Equipment
- P > 10 atm – Cost ↑