

CHEMICAL REACTOR DESIGN FOR PROCESS PLANTS

Volume Two: Case Studies and Design Data

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CASE STUDY 105

Shift Conversion

THIS STUDY illustrates the design of massive adiabatic, catalytic reactors and the use of thermodynamics to set operating conditions. Development of necessary details for a process vessel sketch preliminary to detailed mechanical design is demonstrated.

Problem Statement

Design a shift conversion system for converting the carbon monoxide present in the gas from a reformer of an ammonia plant to carbon dioxide. The following specifications apply. Figure CS-5.1 is a flow diagram for an ammonia plant showing the three major reactors—reformer, shift converter, and ammonia converter.

Feed and Product Specifications

Synthesis gas from the reforming section of an ammonia plant is available at the following conditions:

Feed (Dry Gas Basis): 12,400 lb moles/hr

	Mole %	MW	(%)(MW)
CO	13.0	28	364.0
CO ₂	7.9	44	347.6
H ₂	56.8	2	113.6
N ₂	21.8	28	610.4
CH ₄	0.5*	16	8.0
	100.0		1443.6 $M_m = 14.44$

* Argon included in methane.

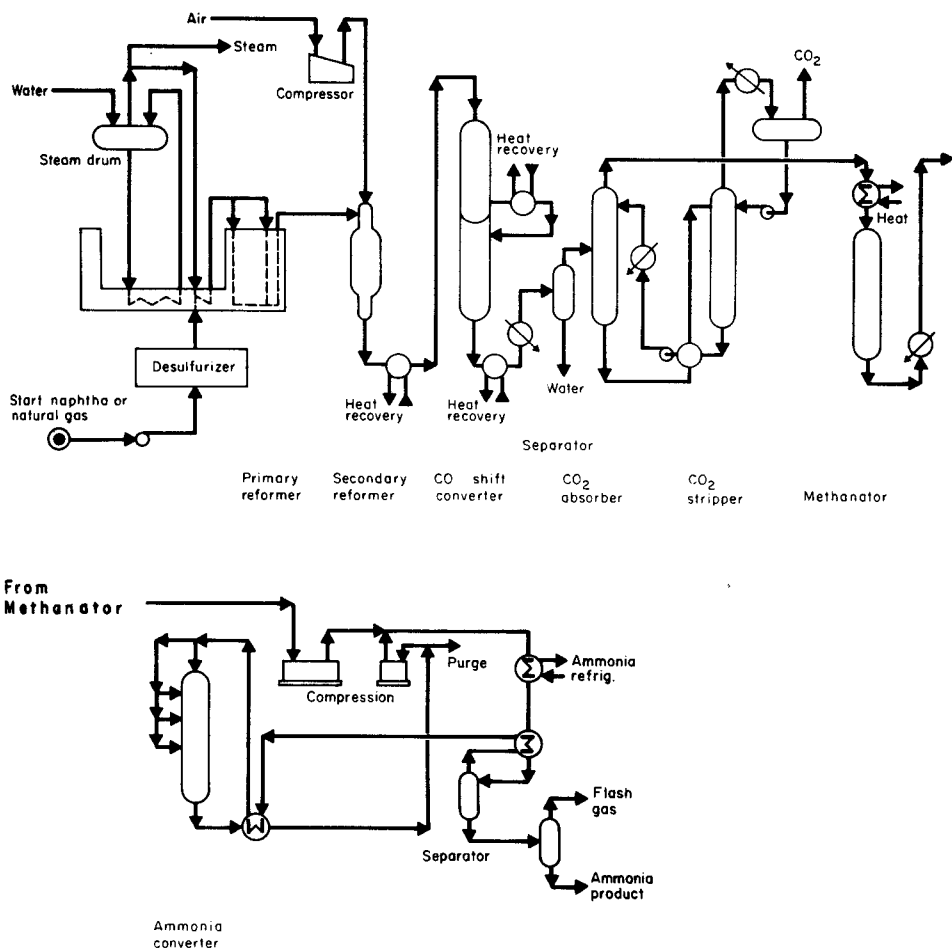


Fig. CS-5.1 Schematic flow diagram for an ammonia complex. Courtesy: The Pullman Kellogg, Division of Pullman, Inc., Houston, Tex.

Total wet feed from reformer: 20,460 lb moles/hr, $M_m = 15.84$.

Reformer discharge conditions: 400 psia, 1750°F.

Impurity specifications: CO—0.2% to 0.5% after shift conversion (dry gas basis) is a typical range. Value selected depends on steam-to-CO ratio and other factors.

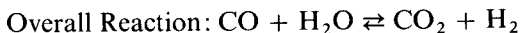
Fuel cost basis: \$0.50/MM BTU.

Catalysts

Two catalysts are available for the shift conversion, chromia-promoted iron catalyst, which has been used many years for the shift reaction, and a copper-zinc catalyst that offers the thermodynamic advantage of lower operating temperatures for this exothermic reaction. Additional catalyst data are given in the following:

Type	Chromia-promoted iron oxide	copper-zinc oxide
Maximum operating temp., °F	890	500–550
Tablet size (in.)	$\frac{1}{4} \times \frac{1}{4}$	$\frac{1}{4} \times \frac{1}{8}$
Bulk density (lb/cu ft)	70	90
Particle density (lb/cu ft)	126	155
Cost (\$/cu ft)	20.00	75.00
Catalyst poisons	Inorganic salts, boron, oils, or phosphorous compounds, liquid H ₂ O is a temporary poison. Sulfur compounds in an amount greater than 50 ppm	Sulfur and halogen compounds, and un- saturated hydro- carbons
Catalyst life	3 yr and over depending on care in startup and opera- tion (Use times up to 15 yr have been reported)	2–3 yr

Chemistry and Kinetics



The iron-oxide catalyst has been studied in greater detail (1). CO is apparently chemisorbed on the iron oxide and both water and CO₂ are strongly adsorbed. CO₂ has an inhibiting effect on the forward rate, and hydrogen appears not to be adsorbed. There are no significant side reactions.

Various manufacturers suggest rate equations for their catalysts. One such manufacturer recommends the following which will be assumed to represent midlife activity (2):

$$(-r_{\text{CO}}) = \psi k (y_{\text{CO}} y_{\text{H}_2\text{O}} - y_{\text{CO}_2} y_{\text{H}_2} / K) / (379 \rho_b) \quad (\text{CS-5.1})$$

where k = rate constant

= $\exp(15.95 - 8820/T)$ for iron catalyst

= $\exp(12.88 - 3340/T)$ for copper-zinc catalyst

K = equilibrium constant

= $\exp(-4.72 + 8640/T)$ for $760 \leq T \leq 1060$

= $\exp(-4.33 + 8240/T)$ for $1060 \leq T \leq 1360$

P = pressure, atm

$(-r_{\text{CO}})$ = rate, lb moles CO converted/(lb catalyst)(hr)

T = temperature, °R

y_j = mole fraction of component indicated

ρ_b = catalyst bulk density, lb/cu ft

ψ = activity factor

Iron catalyst $\psi = 0.816 + 0.184P$ for $P \leq 11.8$

= $1.53 + 0.123P$ for $11.8 < P \leq 20.0$

= 4.0 for $P > 20.0$

Copper-zinc catalyst $\psi = 0.86 + 0.14P$ for $P \leq 24.8$

= 4.33 for $P > 24.8$

Anyone seeking confirming evidence of the efficacy of rate equations in predicting plant performance will certainly find that equations recommended by catalyst manufacturers have been subjected to numerous tests, including many observations on full-scale plants. The rate constants are expressed on the basis of a reasonable "lined-out" activity that the catalyst would maintain for a considerable time provided operating errors which cause deactivation do not occur. We will assume that this equation represents activity levels characteristic of mid-life of the catalyst.

Extensive investigations on the iron catalyst, as discussed on p. 150¹, confirm the form of Eq. CS-5.1 and the ψ term is shown to be the product of the total pressure in atmospheres and ratio of the first-order constant at pressure P to that at atmospheric pressure and is a function of pressure and the Thiele modulus, as shown in Eq. 3.47, p. 153¹. The manufacturer's recommended equation for ψ closely approximates values obtained from Eq. 3.47.

Thermodynamics

Equilibrium CO mole fraction and adiabatic reaction temperature plots are presented in Fig. CS-5.2 based on the following equations.

Ideal molal gas heat capacity equations are adequate since for this system $c_p - c_p^*$ is negligible. The following equation and constants were used (4).

$$c_{p_j} = a + bT + cT^2 + dT^3, T = ^\circ\text{K} \quad (\text{CS-5.3})$$

	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
CO	6.726	+0.04001	+0.1283	-0.5307
H ₂ O	7.7	+0.04594	+0.2521	-0.8587
CO ₂	5.316	+1.4285	-0.8362	+1.784
H ₂	6.952	-0.04567	+0.09563	-0.2079
N ₂	6.903	-0.03753	+0.1930	-0.6861
CH ₄	4.75	+1.2	+0.303	-2.63

Quite obviously an adiabatic reactor is possible, for the changes in temperature are modest particularly at high steam ratios which are needed to improve the equilibrium because of the large amount of hydrogen in the feed. The heat generation potential is also quite low (1.12, see Table 6.4). The steam minimizes temperature change by increasing the heat capacity of the system.

It is clear from Fig. CS-5.2 that when assuming an optimum equilibrium approach temperature of 50°, as recommended for this system, the desired reduction in CO cannot be attained with the iron catalyst when operating in the range of 750°F (100° less than maximum allowable). By operating at 400°F with the copper-zinc catalyst (100° less than its maximum allowable) it is possible to attain the desired reduction in CO, but this catalyst is more expensive. Three alternates are possible.

1. Remove part of CO with iron catalyst in one bed. Then absorb CO₂ and go to a second bed of the same catalyst with a more favorable equilibrium since the product CO₂ is absent.
2. Conduct the entire reaction in a single bed on zinc-copper catalyst.
3. Remove part of the CO in a bed with iron catalyst and complete the removal in a second bed of the more expensive copper-zinc catalyst.

The second and third alternates will be considered as the most attractive if for no other reason than additional absorption equipment creates added maintenance problems particularly because of the corrosive character of monoethanolamine, the usual absorbent.

Design Conditions

General decisions on operating conditions are now possible.

Pressure

Since pressure increases the reaction rate, the shift convertor should operate at the reformer pressure less the drop through the waste-heat boiler after the secondary reformer and associated piping (~ 10 psi). Pressures of 390 psia for first reactor and 380 psia for second will be used.

Steam-to-CO Ratio

Steam-to-CO ratios must surely be in the range of 4 : 1 or higher as indicated by Fig. CS-5.2. The optimum value can only be determined by economic analysis based on design studies. On the negative side higher steam rates cause greater flows and larger diameter equipment. Since steam is also required for the secondary reformer (Fig. CS-5.1), there is substantial logic in adding all needed steam at that point. The recoverable heat is in a more valuable form, and the reformer equilibria are also favorably influenced. Alternatively, additional steam might be injected as quench for the secondary reformer in lieu of a waste heat boiler. This particular case study would normally be conducted as part of a general design study for the entire ammonia plant, and the effects of changes on the total economics assessed. The feed stream given has a ratio of 5 : 1 steam-to-CO, which is quite adequate for the shift reaction. Referring to Fig. CS-5.2 even a 12 : 1 ratio at 500°F feed temperature will not accomplish the desired removal in one stage with the high-temperature catalyst.

If an upper limit of 450°F is to be maintained for the low temperature catalyst, it is clear from Fig. CS-5.2 that the second alternate, a system with all low-temperature catalyst is not feasible. The required inlet temperature of 279°F would be below the dew point of the feed (see the following). Thus only alternate 3 remains to be considered.

Temperature and Outlet CO Concentration

A minimum inlet temperature must be established relative to the dew point. Contact of either catalyst with liquid water at operating temperatures will cause thermal shock and disintegrate the catalyst. An approximate dew point may be estimated as follows: First converter:

$$\begin{aligned}\text{Partial pressure of steam} &= \frac{20,460 - 12,400}{20,460} (390) \\ &= 154 \text{ psi}\end{aligned}$$

Corresponding temperature of saturated steam is 361°F. First converter inlet will be substantially above this value. Assume for purposes of this estimate that 85 % of CO will be removed in first reactor. Hence

$$\begin{aligned}\text{Inlet second converter} &= \frac{20,460 - (12,400)[1 + (0.13)(0.85)]}{20,460} (380) \\ &= 127 \text{ psi}\end{aligned}$$

Corresponding saturated steam temperature is 345°F. Therefore, design for minimum inlet temperature of around 25° above 345°F, approximately 370°F at inlet of secondary reactor.

The maximum temperatures of 890 and 550°F, respectively, for the two catalysts should be used for vessel mechanical design, but process design should be based on a lower temperature. Thus the outlet temperatures must be less than these values and such that the desired residual CO can be reached.

The manufacturer recommends a 50° approach to equilibrium. Based on Eq. 11.37, p. 528¹, the value is 100°F, but the manufacturer's suggestion will be used, and cases will be selected on both sides of this value to minimize the catalyst requirements.

Referring to Fig. CS-5.2 in the low temperature region, it is clear that based on a 50° approach and 5:1 steam-to-CO ratio that catalyst performance at mid-life of 0.35 % CO in the outlet would require a 450°F outlet. This seems a reasonable temperature around which to structure cases since it is sufficiently removed from the maximum allowable of 500–550°F. By following an adiabatic line back to 400°F we see that a reasonable inlet range (outlet from first reactor) is 3.5 % or less. Using a value of 3.0 % with a 50° approach brings us to an 820°F outlet for the first reactor. It seems reasonable to study values at 3.0 % and below, since higher values will leave little safety factor from the 890°F and place the inlet to reactor no.2 closer to the dew point region.

Referring to the equations for the rate constants for both catalysts, it can be shown that the rate doubles for a rise of 100° for the iron catalyst and 200° for the copper-zinc catalyst. Thus using 790°F as an approximate maximum for design, one has the opportunity to raise the temperature to compensate for a 50 % loss in activity for the iron catalyst. In the case of the low-temperature catalyst it is not possible to set the outlet temperature much less than 450°F.

Since the rate data are based on activities at mid-life, the unit will perform better than design at the outset and can be kept at design outlet CO values by altering temperature strategy as the activity declines toward the last half of its life. Toward the end of this period, however, temperature increases may no longer be effective because the approach to equilibrium will become too close and higher outlet CO concentrations will have to be accepted.

Design Cases

Two-Stage System (5 : 1, steam: CO):

1. Calculate minimum catalyst requirements for the following cases which were selected in the range of the outlet CO previously specified.

CO Outlet Conc. %	Inlet Temp., °F
2.25	600, 610, 620, 630, 640, 650, 670
2.65	630, 640, 650, 664, 670, 680, 700
3.0	650, 660, 670, 680, 700, 710, 720

2. Calculate the second stage for convenience starting at 3.0% and ending at 0.2%, so that intermediate inlet and outlet values may be selected as desired.

Inlet temperatures: 370 and above.

Design Procedure

Component mole balance

$$\Delta W(-r_{\text{CO}}) = (-\Delta \mathcal{F}_{\text{CO}}) \quad (\text{CS-5.4})$$

$$\mathcal{F}_{\text{CO}_{i+1}} = \mathcal{F}_{\text{CO}_i} - (-\Delta \mathcal{F}_{\text{CO}}); \mathcal{F}_{\text{CO}_{2i+1}} = \mathcal{F}_{\text{CO}_{2i}} + \Delta \mathcal{F}_{\text{CO}_2}, \text{ etc.}$$

where i designates increment number.

Heat Balance. It is convenient to base the heat of reaction on the known inlet temperature of the increment.

$$\begin{aligned} \sum \mathcal{F}_j c_{p_j} (T_{i+1} - T_i) &= (-r_{\text{CO}})(-\Delta H_{\text{CO}})_{T_i} \Delta W \\ &= (-\Delta \mathcal{F}_{\text{CO}})(-\Delta H_{\text{CO}})_{T_i} \end{aligned} \quad (\text{CS-5.5})$$

Algorithm

1. Calculate $(-r_{\text{CO}})$ at inlet conditions to increment, i .
2. Calculate $(-r_{\text{CO}})_{\text{avg}} = (-r_{\text{CO}})_i + [(-r_{\text{CO}})_i - (-r_{\text{CO}})_{i-1}]/2$ (skip for $i = 0$).
3. Calculate new flow rates: $\mathcal{F}_{i+1} = \mathcal{F}_i \pm (-r_{\text{CO}})\Delta W$
4. Calculate c_p and $(-\Delta H_{\text{CO}})$ @ T_i
5. Calculate ΔT from Eq. CS-5.5.
6. $T_{i+1} = T_i + \Delta T$
7. $y_{i+1} = \mathcal{F}_{i+1}/(\mathcal{F}_T)_i$

An increment of 1° can be used and $(-\Delta\mathcal{F}_{\text{CO}})$ calculated from Eq. CS-5.5. The mole fraction of each component is calculated and the percentage of CO in the dry gas at the outlet of the increment. An average rate is then calculated based on inlet and outlet conditions of the increment using Eq. CS-5.1. Then ΔW is determined from Eq. CS-5.4. Then proceed to the next increment until the desired outlet CO concentration.

8. Mole fraction CO in dry gas = $[y_{\text{CO}}/(1 - y_{\text{H}_2\text{O}})]_{i+1}$.

9. Go to Step 1.

Note. A ΔW increment of 200 lb was found to never cause a ΔT greater than 1° . The average time for a case was 1 sec, and thus there was no need to change this increment size. Alternatively, one could select an increment size of 1° and calculate ΔX from a heat balance, then ΔW .

Results

The results of the several design cases are summarized in Fig. CS-5.3, where it may be seen that in most cases the optima are not overly sensitive to temperature. It, therefore, becomes an easy task to select a reasonable distribution between the duties of the two reactors by comparing the combinations shown in Table CS-5.1. Outlet temperatures exceeding 790°F for the first reactor and 450°F for the second by more than 5° are excluded.

Design decision obviously depends greatly on catalyst life. If the assumed life of each catalyst is correct, case 2 is slightly preferred over case 1. The choice between various outlet CO concentrations in dry gas for reactor no. 2

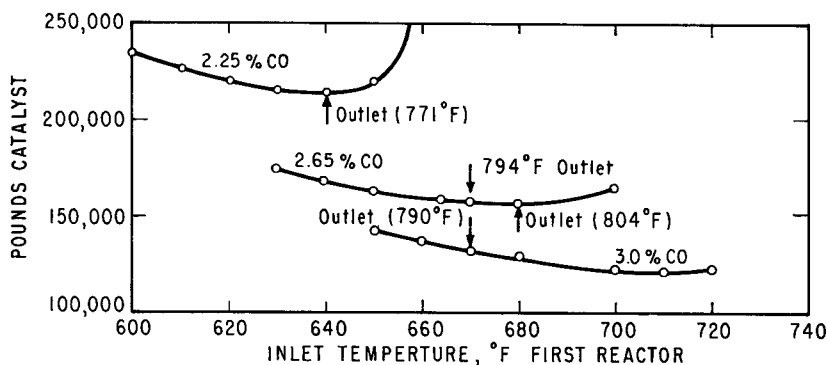


Fig. CS-5.3 Catalyst requirements as function of inlet temperature and outlet CO (first reactor only, 5: 1 steam-to-CO with CO percent at outlet shown).

Table CS-5.1 Results of Calculations

Reactor No.	Outlet CO, %	Temperature, °F		Pounds of Catalyst	Cost of Catalyst, \$ ^a	4-Yr Cost, \$
		In	Out			
Case 1:						
# 1	2.25	640	771	215,800	61,657	
# 2	0.3	400	429	150,040	125,033	
Total					186,690	311,725
# 1	2.25	640	771	215,800	61,657	
# 2	0.35	421	448.3	131,750	109,792	
Total					171,449	281,241
# 1	2.25	640	771	251,800	61,657	
# 2	0.40	421	447.5	116,900	97,417	
Total					159,074	256,491
Case 2:						
# 1	2.65	670	794	157,700	45,057	
# 2	0.2	370	400	205,400	171,500	
Total					216,557	388,057
# 1	2.65	670	794	157,700	45,057	
# 2	0.3	395	429	160,100	133,417	
Total					178,474	311,891
# 1	2.65	670	794	157,700	45,057	
# 2	0.35	415	448	141,230	117,692	
Total					162,749	280,441
# 1	2.65	670	794	157,700	45,057	
# 2	0.4	425	457.5	126,140	105,117	
Total					150,174	255,291
Case 3:						
# 1	3.0	670	790	132,229	37,780	
# 2	0.3	400	439	167,600	139,467	
Total					177,447	317,114
# 1	3.0	670	790	132,229	37,780	
# 2	0.35	410	448	148,330	123,608	
Total					161,388	284,996
# 1	3.0	670	790	132,229	37,780	
# 2	0.4	420	457.5	133,000	110,833	
Total					148,613	259,446

^a Basis: Catalyst Life Reactor No. 1, 4 yr.
Catalyst Life Reactor No. 2, 2 yr.

remains. As the outlet CO increases more CO must be converted to CH_4 in the methanator, which increases the inerts concentration in the synthesis loop and decreases the ammonia production: For our purposes an approximate rule-of-thumb will be used:

For each 0.1 % increase in inerts there is a 1 % decline in ammonia production.

This fact provides much incentive for maintaining low CO concentrations at the outlet of reactor no. 2. Within these low ranges the decline in production can be offset by modest operating changes at the ammonia converter. An increase in operating pressure can offset the decline in rate caused by the lower reactant partial pressure created by the added inerts. Based on some reasonable steam costs for the plant being considered and turbine water rates, a cost of \$16,500/yr for each increase of 0.1 % CO has been estimated. This value will be useful for illustrative purposes, but in a real case actual design calculations on the ammonia converter will yield a more precise value.

Four-year incremental costs of case 2 can be summarized for catalyst and energy with an arbitrary basis of zero for energy at 0.2 % CO and for catalyst at 0.4 % CO.

% CO	Incremental 4-year Costs*
0.2	\$132,766
0.3	\$122,600
0.35	\$124,150
0.40	\$132,000

Again, the optimum is flat, and it seems best to select a catalyst charge and outlet CO that will provide good operating flexibility. Since the rate equations are based on used catalyst, early operation will yield low CO values and performance toward the end of the run will produce high CO values. By placing the design on the middle of this region operating flexibility is obtained along with that already provided for raising the temperature.

Decision. 1. Size reactor volume on basis of catalyst required for 0.3 % CO. Table CS-5.2 summarizes the operating conditions.

* The results are dramatically altered using 1977 costs (\$1.80/MM BTU for energy and \$110/cu ft for cat. # 2, an increase of 260% for energy and only 47% for catalyst). Operation at 0.2% will now be definitely favored. The incremental 4-year costs are \$194,723 for 0.2% CO, \$320,701 for 0.3% CO, \$393,213 for 0.35% CO, and \$475,200 for 0.4% CO.

Table CS-5.2 Summary of Operating Conditions for Reactors No. 1 and No. 2

Reactor no. 1

Inlet pressure: 26.53 atm (10 psi drop for waste heat boiler and piping)

Inlet temperature: 670°F

Outlet temperature: 794°F

CO in dry gas: 13.0% in, 2.65% out

Catalyst: 157,700 lb (2253 cu ft)

Reactor no. 2

Inlet pressure: 25.85 atm (10 psi drop between inlet of # 1 and inlet of # 2 allowed)^b

Inlet temperature: 415°F

Outlet temperature: 448°F

CO in dry gas: 2.65% in, 0.30% out

Catalyst (based on 0.3% CO): 160,100 lb (1789 cu ft)

Compositions (dry gas)

Component	Mole %		
	Inlet # 1	Outlet # 1 Inlet # 2	Outlet # 2
CO	7.879	1.77	0.24
H ₂ O	39.394	33.28	31.75
CO ₂	4.788	10.90	12.43
H ₂	34.424	40.54	42.07
N ₂	13.212	13.212	13.212
CH ₄	0.303	0.303	0.303
	100.000	100.000	100.000

Average viscosity, cp^a

In 0.0242

Out 0.0262

 c_{pm} (In) 7.98 (Out) 7.87

Total Flow: 20,460 lb-moles/hr.

Average MW: 15.84.

^a Based on mixture method in *API Data Book*.^b Includes ΔP for boiler feedwater exchanger.

2. Base other calculations and material balance on 0.35% CO so that additional capacity will be provided in all downstream equipment.

Reactor Configuration

Based on reactor inlet conditions (Table CS-5.2) determine mass flow rate that will minimize temperature and concentration gradients between fluid phase and catalyst surface without excessive pressure drop.

Reactor No. 1 @ 670°F and 26.53 Atm

Using Fig. 11.5 and Table CS-5.2

$$N_{Re} = \frac{d_p G}{\mu} = \frac{(1.225)(0.25)G}{(12)(0.0242)(2.42)} = 0.436G$$

$$a_m = \frac{6}{D_p \rho_p} = \frac{(6)(12)}{(0.25)(126)} = 2.286 \text{ ft}^2/\text{lb}$$

$$\begin{aligned} (-r_{CO}) &= \psi k(y_{CO} y_{H_2O} - y_{CO_2} y_{H_2}/K)/379 \rho_b \\ &= (4) \frac{3550}{(379)(70)} \left[(0.79)(0.394) - \frac{(0.048)(0.344)}{19.4} \right] \\ &= 0.0161 \end{aligned}$$

$$R_m = \frac{(-r_{CO})M_m}{a_m G} = \frac{(0.0161)(15.84)}{(2.286)G} = \frac{0.112}{G}$$

$$q_m = R_m \frac{(-\Delta H)}{(c_{pm})} = \frac{(0.112)(9280)}{7.98G} = \frac{130}{G}, ^\circ\text{C}$$

From Fig. 11.5 it is apparent that G values 500 and above meet the ΔT requirements. There is no need to calculate the Prandtl number. A value of 1.0 is conservative. To avoid calculating a Schmidt number, use a conservative value of 5 for which $\Delta y_i \sim 0.006$ at these mass velocities. This is less than 10% of limiting reactant mole fraction.

Pressure Drop (Reactor No. 1)

From Eqs. 11.7 and 11.8B at average of inlet and outlet,

$$N_{Re} = \frac{D_p G}{\mu} = \frac{(0.25)G}{(12)(0.025)(2.42)} = 0.344G$$

$$\begin{aligned} f_k &= 1.75 + 150 \frac{(1 - \varepsilon)}{N_{Re}} \\ &= 1.75 + 150 \frac{0.555}{0.344G} = 1.75 + \frac{242}{G} \end{aligned}$$

For $G = 500$, $f_k = 2.23$

$$\begin{aligned} \frac{\Delta P}{\Delta L} &= \frac{f_k G^2}{D_p \rho_t g_c} \left(\frac{1 - \varepsilon}{\varepsilon^3} \right) \\ \Delta P/\text{ft} &= \left[\frac{(2.23)(500)^2}{(0.25/12)(0.483)(32.17)(3600)^2} \right] \left[\frac{0.555}{(0.445)^3} \right] \\ &= 0.837 \text{ psf/ft or } 5.8 \times 10^{-3} \text{ psi/ft} \end{aligned}$$

Can use higher G to reduce equipment size.

Table CS-5.3 *L/D Study for Reactor No. 1 (1971 Costs)*

$D \times L$, ft ^a	Thickness in.	Bed Height, ft	G	ΔP , psi	Vessel Weight, lb	Vessel Cost, ^b \$	Inert Support		Total \$	Savings		Net Savings \$
							ft ^{3c}	\$		Vessel Δ \$	Compression Δ \$ ^d	
14 × 19	3.19	14.63	2100	1.26	173,000	114,180	360	3380	117,560	0	0	
13 × 21	2.97	16.97	2440	1.95	156,600	104,874	288	2710	107,584	9,974	(-2,524)	7,450
12 × 24	2.75	19.92	2860	3.12	142,300	98,187	226	2220	100,407	17,153	(-8,077)	9,076
11 × 28	2.53	23.72	3400	5.21	131,400	93,819	174	1640	95,459	22,101	(-17,668)	4,433
10 × 33	2.31	28.70	4130	9.23	121,800	88,914	131	1230	90,144	27,416	(-36,850)	(-9,434)
9 × 40	2.09	35.41	5080	17.13	114,200	84,508	96	900	85,408	32,152	(-75,718)	(-43,566)

^a Approximately 4 ft added to length in order to account for inert material between tangents at top and bottom and for free space above bed for distributor and work area.

^b See Appendix B for example calculation. Costs for this type vessel varied from 66 ¢/lb at 14 ft to 74 ¢/lb at 9 ft diameter at time of calculation. ASTM A387D (2¼ Cr-1 Mo) selected for resistance to hydrogen attack (Fig. B.1 Appendix).

^c Amount of inert support varies with volume of bottom head (¾ in. × 7/8 in. pellets @ \$9.40/cu ft).

^d Compressor delta operating costs are affected lower suction pressure on first-stage of synthesis-gas compressor caused by increased ΔP in bed. Costs are calculated as shown in the Appendix C on the basis of 50 ¢/MM BTU fuel gas and 4 yr payout.

VESSEL SPECIFICATION SHEET				ITEM NO. <u>R-101</u>	
CUSTOMER _____				JOB NO. _____	
SERVICE OF UNIT <u>FIRST-STAGE SHIFT CONVERTER</u>				REV. _____ DATE _____	
NO. REQ'D <u>1</u> SIZE: <u>12'-0" I.D. x 24'-0" TT</u>				PREPARED BY _____ DATE _____	
CONSTRUCTION				CHECKED BY _____ DATE _____	
CODE: <u>ASME Sect. VIII Div. I</u> STAMP: <u>Yes</u>				APPROVED _____ DATE _____	
PRESS. (PSIG) <u>MAX OP 390</u> NOR. OP. <u>390</u> DESIGN: <u>467</u>				PLANT _____	
TEMP. (°F) <u>MAX OP 850</u> NOR. OP. <u>794</u> DESIGN: <u>890</u>					
WIND VELOCITY: <u>100</u> MPH CORR. ALLOW: <u>1/8</u>					
STRESS RELIEVE: _____ X-RAY <u>Yes</u>					
PHYS. & CHEM. TESTS: _____					
Calculated Thickness : <u>2.75 in. (Includes corr. all)</u>					
MATERIAL	SPEC	MATERIAL	SPEC		
SHELL ASTM	A 387 D	INTERALS			
HEADS	A 387 D	DAVIT/HINGE			
SUPPORTS		PLATFORMS			
FLANGES	A 182 Gr F22	LADDER (CAGED)			
PIPE	A 335 P22	CLIPS			
COUPLINGS		PAINTER TROLLEY			
GASKETS		LIFTING LUGS			
BOLTS		PAINT			
NUTS		INSULATION			
NOZZLE SCHEDULE					
MK.	SERVICE	NO.	SIZE	RATING	FACING
N-1	Manway & Inlet	1	20"	400 #	
N-2	Outlet	1	20"	"	
N-3	Catalyst Discharge	1	12	"	
N-4	Thermowells	4			
N-5					
N-6					
N-7					
N-8					
N-9					
N-10					
N-11					
N-12					
N-13					
N-14					
N-15					
M-1	MANHOLE				
REMARKS:					
* Evenly spaced over catalyst bed					
SKIRT OPENINGS:					

Fig. CS-5.4 Process vessel sketch for reactor 1, shift converter.

Reactor L/D Selected and Final Design

The reactor L/D selected above $G = 500$ will depend on minimizing the reactor cost plus incremental compression costs produced by reactor ΔP . A summary for various L/D ratios at constant volume based on the required catalyst is given in Table CS-5.3 for reactor no. 1 and a process vessel sketch is shown in Fig. CS-5.4. The 12-ft diameter reactor was selected as most economical.

Similar calculations for reactor no. 2 were also carried out which resulted in selecting a reactor 12 ft in diameter by 20 ft tangent-to-tangent.

Other Appurtenances

Because of the high sensitivity of the low-temperature catalyst to sulfur poisoning, a guard bed is placed on top of the catalyst bed. The height for good distribution is simply set at 100 times the particle diameter of $\frac{1}{4}$ in., or 2 ft. Guard materials have been reported with long life times (3). These include zinc oxide and special guard solids which also protect against chloride poisoning of the catalyst.

An attractive alternate arrangement for the second converter, though requiring greater capital expenditure, would be two parallel reactors each 8 ft in diameter and 20 ft tangent-to-tangent. Costs could be minimized by mounting one above the other with a common header between them. As the catalyst deactivated one bed could be replaced while the other remained operative without excessive loss of ammonia production. At a wholesale price of \$30/ton of NH_3 , total shutdown of a plant this size is most costly. The decision must be made on the total economics of the ammonia complex, which is beyond the scope of this particular illustrative case.

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