PROJECT 5

Problems at the Cumene Production Facility, Unit 800

C.5.1 BACKGROUND

Cumene (isopropyl benzene) is produced by reacting propylene with benzene. During World War II, cumene was used as an octane enhancer for piston engine aircraft fuel. Presently, most of the worldwide supply of cumene is used as a raw material for phenol production. Typically, cumene is produced at the same facility that manufactures phenol.

The plant at which you are employed currently manufactures cumene in Unit 800 by a vapor-phase alkylation process that uses a phosphoric acid catalyst supported on kieselguhr. Plant capacity is on the order of 90,000 metric tons per year of 99 wt% purity cumene. Benzene and propylene feeds are brought in by tanker trucks and stored in tanks as a liquid.

C.5.2 CUMENE PRODUCTION REACTIONS

The reactions for cumene production from benzene and propylene are as follows:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \rightarrow \underset{p\text{-diisopropyl benzene}}{C_{12}H_{18}}$$

C.5.3 PROCESS DESCRIPTION

The PFD for the cumene production process, Unit 800, is given in Figure C.8. The reactants are fed from their respective storage tanks. After being pumped up to the required pressure (dictated by catalyst operating conditions), the reactants are mixed, vaporized, and heated in the fired heater to the temperature required by the catalyst. The shell-and-tube reactor converts the reactants to desired and undesired products as per the

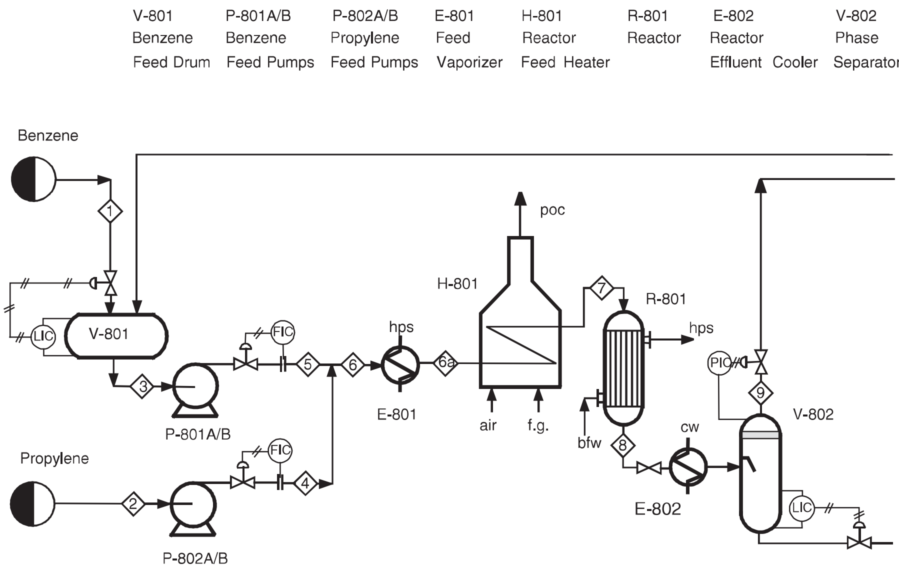


Figure C.8 Process Flow Diagram for the Production of Cumene Process (Unit 800)

above reactions. The exothermic heat of reaction is removed by producing high-pressure steam from boiler feed water in the reactor. The stream leaving the reactor enters the flash unit, which consists of a heat exchanger and a flash drum. The flash unit is used to separate the C_3 impurities, which are used as fuel for a furnace in another on-site process. The liquid stream from the flash drum is sent to the first distillation column, which separates benzene for recycle. The second distillation column purifies cumene from the p-diisopropyl benzene (p-DIPB) impurity. Currently, the waste p-DIPB is used as fuel for a furnace. The pressure of both distillation columns is determined by the pressure in the flash drum; that is, there are no pressure-reduction valves downstream of the flash drum.

C.5.4 RECENT PROBLEMS IN UNIT 800

Recently, Unit 800 has not been operating at standard conditions. We have recently switched suppliers of propylene; however, our contract guarantees that the new propylene feed will be within specifications given in Table C.13.

Upon examining present operating conditions, we have made the following observations:

1. Production of cumene has dropped by about 8%, and the reflux in T-801 was increased by approximately 8% in order to maintain 99 wt% purity. The flows of benzene (Stream 5) and propylene (Stream 2) remained the same. Pressure in the

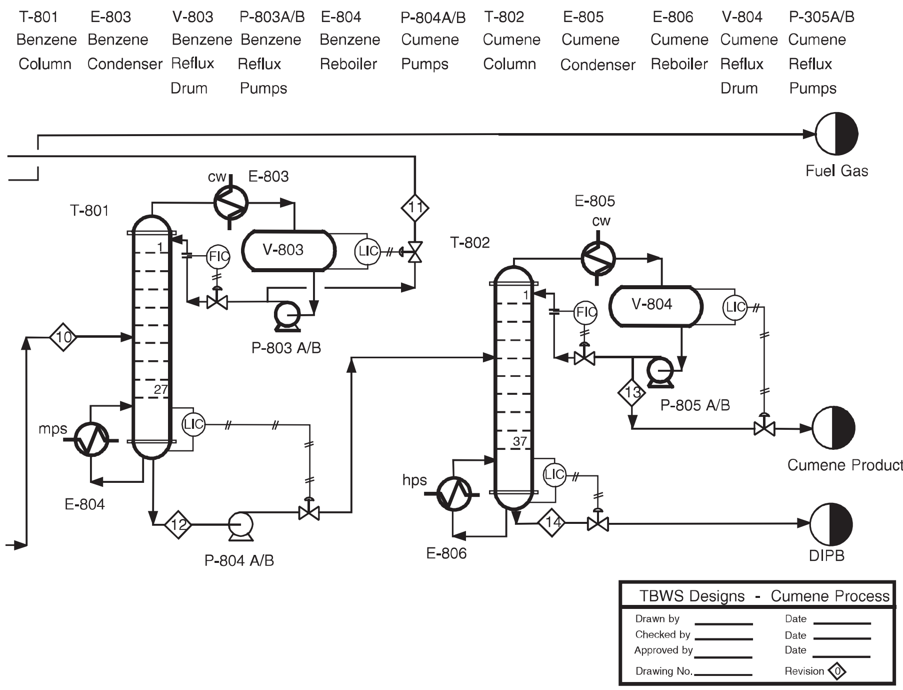


Figure C.8 (*Continued*)

storage tanks has not changed appreciably when measured at the same ambient temperature.

2. The amount of fuel gas being produced has increased significantly and is estimated to be 78% greater than before. Additionally, it has been observed that the pressure control valve on the fuel gas line (Stream 9) coming from V-802 is now fully open, although previously it was controlling the flow.
3. The benzene recycle, Stream 11, has increased by about 5%, and the temperature of Stream 3 into P-801 has increased by about 3°C.
4. Production of steam in the reactor has fallen by about 6%.
5. Catalyst in the reactor was changed six months ago, and previous operating history (over last ten years) indicates that no significant drop in catalyst activity should have occurred over this time period.
6. p-DIPB production, Stream 14, has dropped by about 20%.

We are very concerned about this loss in production because we can currently sell all the material we produce.

Another problem that has arisen lately is the malfunction of the feed pumps. This problem arose during a very warm spell when the ambient temperature reached 110°F. A maintenance check showed that P-802 needed a new bearing, and this was taken care of, but P-801 seemed to be OK. The ambient temperature has now returned to a mild 70°F, and both pumps seem to be working fine.

Table C.13 Specifications of Products and Raw Materials

Raw Materials	
Benzene	>99.9 wt% purity
Propylene	≤ 5 wt% propane impurity
Product	
Cumene	>99 wt% purity

Currently, market conditions for cumene are very tight. We are in direct competition with some local companies that have recently built cumene plants. It appears that management is very concerned about our competitiveness because other producers in the area are beginning to undercut our prices. Management wants to find out whether any significant savings in operating costs can be found for Unit 800.

C.5.5 OTHER INFORMATION

Other pertinent information is appended, including a flow table for the process streams at design conditions, that is, prior to the current operating problem, Table C.14; a utility summary table at design conditions, Table C.15; pump curves, Figures C.9 and C.10; a set of design calculations; and an equipment list, Table C.16.

C.5.6 ASSIGNMENT

Specifically, you are to prepare the following by . . . (two weeks from now):

1. A written report detailing your diagnosis of the operating problems with the plant, along with your recommendations for solving these problems
2. A list of new equipment to be purchased, if any, including size, cost, and materials of construction
3. An analysis of any change in the annual operating cost created by your recommended modifications
4. A legible, organized set of calculations justifying your recommendations, including any assumptions made

C.5.7 REPORT FORMAT

This report should be brief. Most of the report should be an executive summary, not to exceed five double-spaced, typed pages, which summarizes your diagnosis, recommendations, and rationale. Figures and tables may be included (do not count these against the page limit) in the executive summary. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. The guidelines given in Chapter 29 (in this CD) should be followed.

Table C.14 Flow Summary Table for Cumene Production at Design Conditions, Unit 800 (Figure C.8)

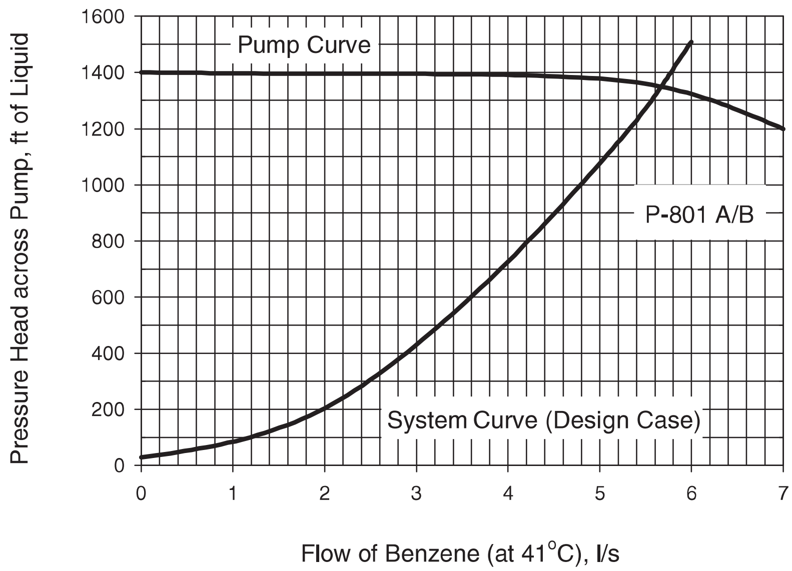
Stream Number	1	2	3	4	5	6	6a	7
Temperature (°C)	25	25	41	28	44	41	214.0	350
Pressure (bar)	1.00	11.66	1.01	31.50	31.50	31.25	30.95	30.75
Vapor mole fraction	0	0	0	0	0.0	0.0	1.0	1.0
Flowrate (tonne/h)	8.19	4.64	16.37	4.64	16.37	21.01	21.01	21.01
Flowrates (kmol/h)								
Benzene	105.00	0.0	205.27	0.0	205.27	205.27	205.27	205.27
Propylene	0.0	105.00	2.89	105.00	2.89	107.89	107.89	107.89
Propane	0.0	5.27	2.79	5.27	2.79	8.06	8.06	8.06
Cumene	0.0	0.0	0.94	0.0	0.94	0.94	0.94	0.94
P-diisopropyl benzene	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total (kmol/h)	105.00	110.27	211.89	110.27	211.89	322.16	322.16	322.16

Stream Number	8	9	10	11	12	13	14
Temperature (°C)	350	90	90	57	179	178	222
Pressure (bar)	30.25	1.75	1.75	1.75	1.90	1.90	2.10
Vapor mole fraction	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Flowrate (tonne/h)	21.01	1.19	19.82	8.18	11.64	11.08	0.56
Flowrates (kmol/h)							
Benzene	108.96	7.88	101.08	100.27	0.81	0.81	0.0
Propylene	8.86	5.97	2.89	2.89	0.0	0.0	0.0
Propane	8.06	5.27	2.79	2.79	0.0	0.0	0.0
Cumene	94.39	0.77	93.62	0.94	92.68	91.76	0.92
P-diisopropyl benzene	2.79	0.0	2.79	0.0	2.79	0.03	2.76
Total (kmol/h)	223.06	19.89	203.17	106.89	96.28	92.60	3.68

Table C.15 Flow Summary Table for Utility Streams in Unit 800

Stream Name	hps to E-801	Condensate from E-801	mps to E-804	Condensate from E-804	hps to E-806	Condensate from E-806
Temperature (°C)	254	254	185.5	185.5	254	254
Pressure (bar)	42.37	42.37	11.35	11.35	42.37	42.37
Flowrate (tonne/h)	7.60	7.60	3.56	3.56	3.25	3.25

Stream Name	cw to E-802	cw from E-802	cw to E-803	cw from E-803	cw to E-805	cw from E-805
Temperature (°C)	30	45	30	45	30	45
Pressure (bar)	5.16	4.96	5.16	4.96	5.16	4.96
Flowrate (tonne/h)	261.30	261.30	85.88	85.88	87.50	87.50



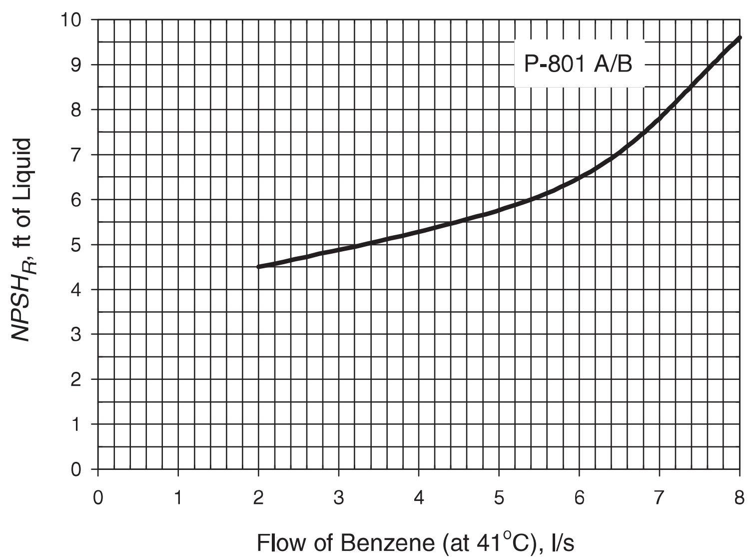


Figure C.9 Pump, System, and NPSH Curves for P-801 A/B

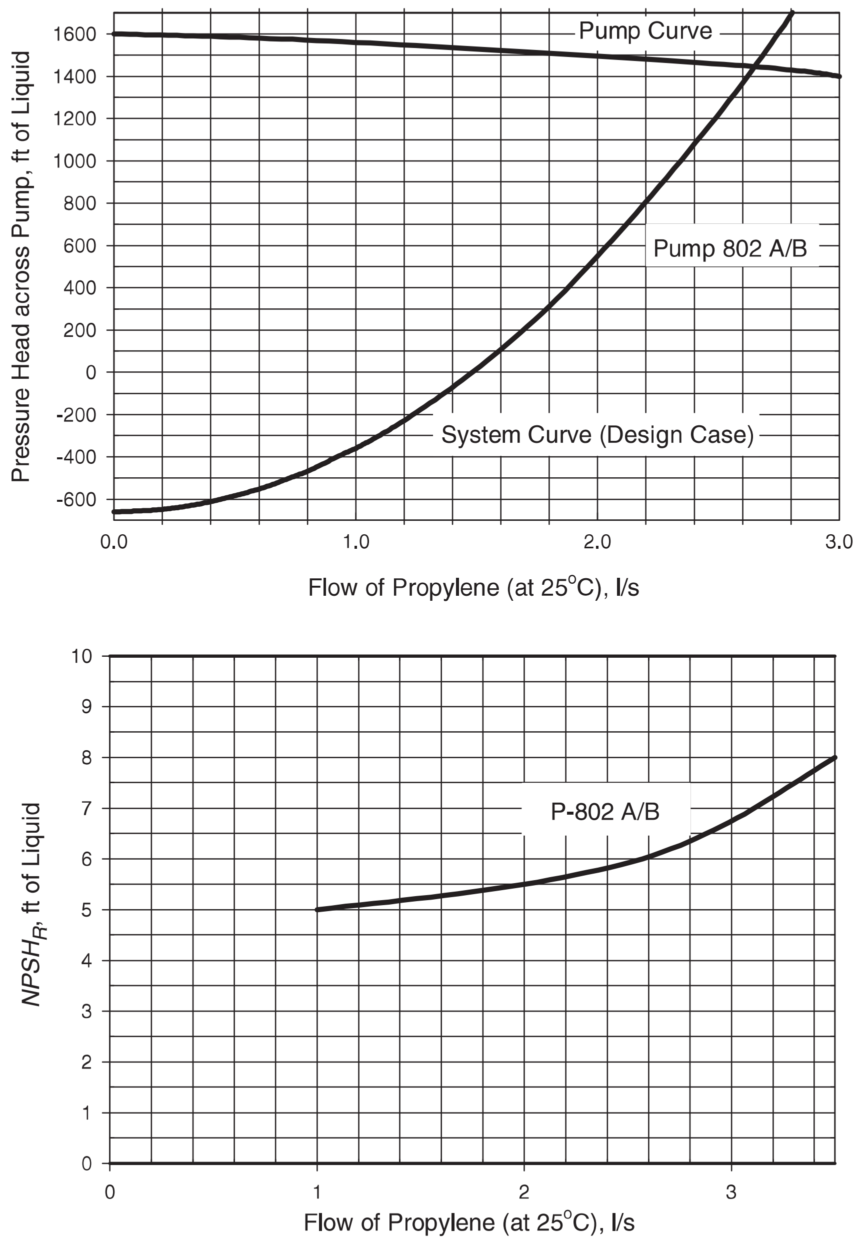


Figure C.10 Pump, System, and NPSH Curves for P-802 A/B

Table C.16 Equipment Summary Table for Unit 800

Tanks (not shown on flowsheet)

TK-801 storage tank for benzene
There are two tanks: one feeding Stream 1 and one in a filling mode.
Each tank is 450 m^3.

TK-802 storage tank for propylene
There are two tanks: one feeding Stream 2 and one in a filling mode.
Each tank is 450 m^3.

Pumps (assume efficiency independent of flowrate)

P-801 centrifugal, 75% efficient, driver rated at 21.9 kW

P-802 centrifugal, 75% efficient, driver rated at 6.8 kW

P-803 centrifugal, 75% efficient, driver rated at 2.4 kW

P-804 centrifugal, 75% efficient, driver rated at 1.0 kW

P-805 centrifugal, 75% efficient, driver rated at 3.3 kW

Heat Exchangers (all one pass on each side, unless otherwise noted; h_i refers to tube side; tube wall resistance negligible, unless otherwise noted)

E-801 uses high-pressure steam, steam in shell, Q = 12,800 MJ/h
A = 20.8 m^2 in two zones
Desubcooling zone: A = 13.5 m^2, U = 600 W/m^2°C, h_i = 667 W/m^2°C
Vaporizing zone: A = 7.3 m^2, U = 1500 W/m^2°C, equal resistances on both sides

E-802 condenser for flash unit, process stream in shell, 1-2 configuration
Q = 16,400 MJ/h, A = 533 m^2

E-803 total condenser for T-801, condensing fluid in shell
A = 151 m^2, U = 450 W/m^2°C, all resistance on water side

E-804 reboiler for T-801
A = 405 m^2, U = 750 W/m^2°C, approximately equal resistances

E-805 total condenser for T-802, condensing fluid in shell
A = 24.0 m^2, U = 450 W/m^2°C, all resistance on water side

E-806 reboiler for T-802
A = 64.0 m^2, U = 750 W/m^2°C, approximately equal resistances

Fired Heater

H-801 Q = 6380 MJ/h (heat actually added to fluid)
Capacity 10,000 MJ/h of heat added to fluid
70% efficiency

Reactor

R-801 shell-and-tube packed bed with phosphoric acid catalyst supported on kieselguhr
Boiler feed water in shell to produce high-pressure steam
Reactor volume = 6.50 m^3, heat exchange area = 342 m^2
234 tubes, 3.0-in (7.62 cm) ID, 6 m long
U = 65 W/m^2°C, all resistance on reactor side
Heat removal required = 9840 MJ/h

Table C.16 Equipment Summary Table for Unit 800 (*Continued*)

Distillation Columns

T-801 removes benzene impurity overhead for recycle
Medium-pressure steam used in reboiler
Cooling water used in condenser, returned at maximum allowable temperature
Reflux ratio = 0.44
27 trays, 50% efficient
24-in tray spacing, 3-in weirs
Diameter = 1.13 m, active area = 75% of total area
Q_c = –5390 MJ/h
Q_r = 7100 MJ/h

T-802 removes cumene product overhead
High-pressure steam used in reboiler
Cooling water used in condenser, returned at maximum allowable temperature
Reflux ratio = 0.63
37 trays, 50% efficient
24-in tray spacing, 3-in weirs
Diameter = 1.26 m, active area = 75% of total area
Q_c = –5490 MJ/h
Q_r = 5520 MJ/h

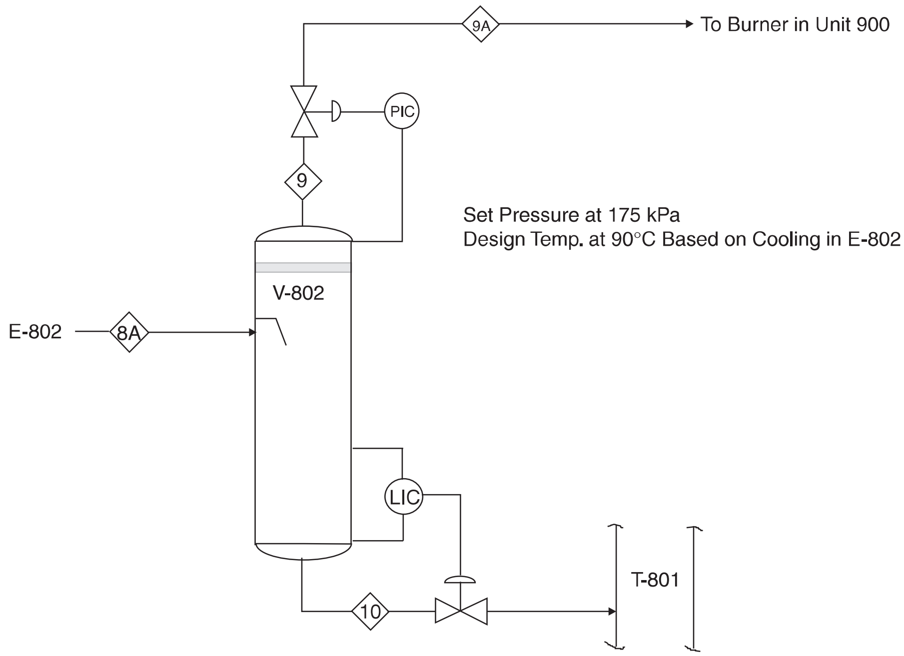
Vessels

V-801	benzene feed drum	4.2 m length, 1.4 m diameter
V-802	flash drum	5.2 m height, 1 m diameter
V-803	T-801 reflux drum	4 m length, 1.6 m diameter
V-804	T-802 reflux drum	6.5 m length, 1.6 m diameter

C.5.8 PROCESS CALCULATIONS

Calculations for Fuel Gas Exit Line for V-802

Design flow of fuel gas = 1192 kg/h
Molecular weight of fuel gas = 59.9
Gas viscosity = 9.5×10^{-6} kg/m.s
Gas density = 1.18 (273) P/(293 + 90) (1.01) = 0.00876P kg/m^3 (P in bar)
Destination pressure (in burner in unit 900) = 1.25 bar
$\Delta P_{line} + \Delta P_{valve} = 1.75 - 1.25 = 0.50$ bar
ΔP_{valve} should be $\cong$ 0.30 bar and $\Delta P_{line} = 0.20$ bar
Length of line (Stream 9A) $\cong$ 125 m (equivalent length including fittings)
Average pressure in line, P = (1.45 + 1.25) / 2 = 1.35 bar
Density of gas in line = 0.00876 P = 1.18 kg/m^3
$\Delta P_{line} = 2f \rho u^2 L_e / d_{pipe}$



Look at 3-in, 4-in, and 6-in schedule-40 pipe:

d_{pipe} (nominal)	3 in.	4 in.	6 in.
$d_{pipe}(\text{inside}) = d_i$	0.0779 m	0.1022 m	0.1541 m
$u = 4Q/\pi d_i^2$	58.9 m/s	34.2 m/s	15.0 m/s
$\text{Re} = u\rho d_i/\mu$	5.69×10^5	4.34×10^5	2.88×10^5
e/d_i	0.00059	0.00045	0.0003
f (from friction factor diagram)	0.0046	0.0045	0.0042
$\Delta P_{line} = \dfrac{2f\rho u^2 L_{eq}}{d_i}$	0.603 bar	0.152 bar	0.018 bar

Choose 4-in schedule-40 pipe.

$$\boxed{\Delta P_{line} = 0.152 \text{ bar and } \Delta P_{valve} = 0.50 - 0.152 = 0.348 \text{ bar}}$$

Calculations for P-801

Design Conditions (note that 1 kPa = 0.335 ft of water = 0.402 ft of benzene)
LAL (low alarm level) = 5 ft from ground and pump center line is 2 ft from ground
NOL (normal operating level) = 10 ft above ground level

NPSH Calculations (at LAL)
Static head = 5 – 2 = 3 ft of benzene = h_{stat}
P_{supply} = 1.01 bar = 40.7 ft of benzene = h_{supply}
$\Delta P_{friction}$ (in supply line) = 1 psi = 2.8 ft of benzene = $h_{friction}$

Vapor Pressure of Stream 3

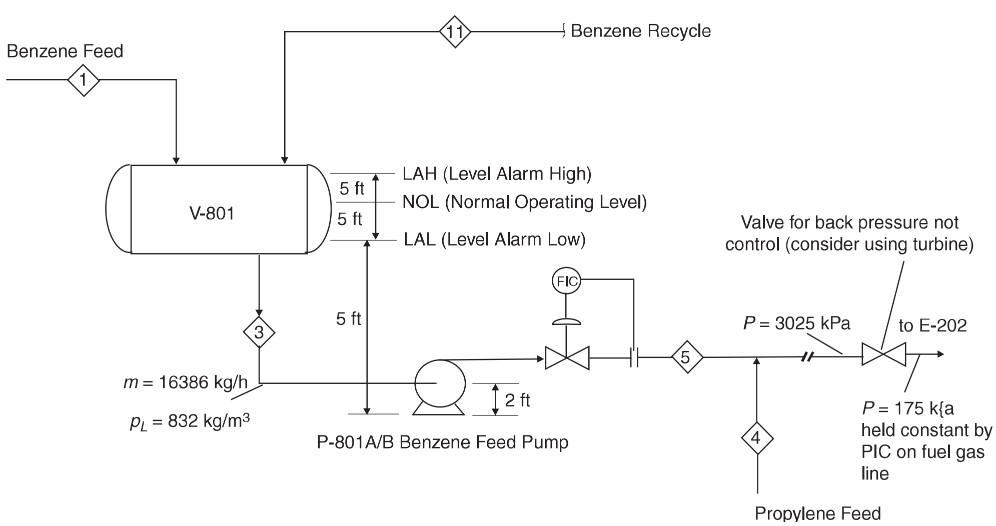
$T = 30°C \quad P^* = 54$ kPa
$T = 40°C \quad P^* = 72$ kPa
$T = 50°C \quad P^* = 94$ kPa

Vapor Pressure of Stream 3 = 0.74 bar @ 41°C = 29.7 ft of benzene = h_{vp}

$NPSH_{available} = h_{supply} + h_{static} - h_{friction} - h_{vp} = 40.7 + 3 - 2.8 - 29.7 = 11.2$ ft
$NPSH_{required}$ (from pump curve) = 6.1 ft @ 5.5×10^{-3} m^3/s
$\therefore$ cavitation should not be a problem

System Curve Calculations

$\Delta P_{friction}$ (discharge) = 31.50 – 1.75 = 29.75 bar = 1196 ft of benzene
$\Delta P_{friction}$ (suction) = 2.8 ft of benzene
$\Delta P_{discharge\text{ - }tank}$ = 1.75 – 1.01 = 0.74 bar = 30 ft of benzene
ΔP_{static} = 0 (E-801 entrance @ 10 ft above ground level = NOL)



$\therefore$ Required head at design flow = 1199 + 30 + ΔP_{cv} = 1230 ft of benzene + ΔP_{cv}
From pump curve this gives us ΔP_{cv} = 135 ft = 3.36 bar (this is high but OK)

Calculations for P-802

Design Conditions (note that 1 kPa = 0.335 ft of water = 0.666 ft of propylene)
LAL (low alarm level) = 10 ft from ground and pump center line is 2 ft from ground
NOL (normal operating level) = 20 ft from ground

NPSH Calculations (at LAL)

Static head = 10 – 2 = 8 ft of propylene = h_{stat}
$P_{supply} = P_{sat}$ (@25°C) = 11.66 bar = 777 ft of propylene = h_{supply}
$\Delta P_{friction}$ (in supply line) = 0.2 psi = 1 ft of propylene = $h_{friction}$ (3-in schedule 40 pipe L_e = 20 ft)

Vapor Pressure of Stream 2 = 11.66 bar = 777 ft of propylene = h_{vp}

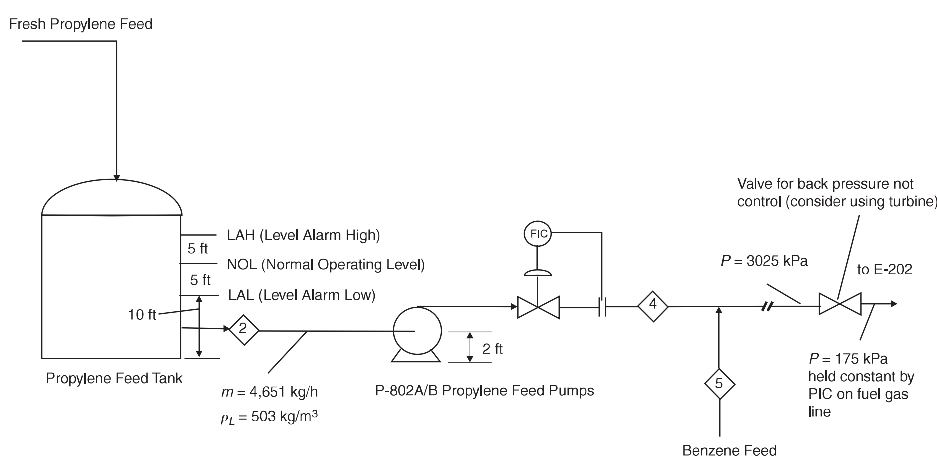
$NPSH_{available} = h_{supply} + h_{static} - h_{friction} - h_{vp}$ = 777 + 8 – 1 – 777 = 7 ft of propylene
(@ propylene flowrate of 2.57×10^{-3} m^3/s)
$NPSH_{required}$ (from pump curve) = 6 ft

$\therefore$ cavitation should not be a problem (put note on P&ID to increase LAL to 12 ft to be safe)

System Curve Calculations

$\Delta P_{friction}$ (discharge) = 31.50 – 1.75 = 29.75 bar = 1981 ft of propylene
$\Delta P_{friction}$ (suction) = 1 ft of propylene
$\Delta P_{discharge\text{-}tank}$ = 1.75 – 11.66 = –9.91 bar = –660 ft of propylene
ΔP_{static} = –10 ft of propylene

$\therefore$ Required head at design flow = 1982 – 660 – 10 + ΔP_{cv} = 1312 ft of propylene + ΔP_{cv}
From pump curve this gives us ΔP_{cv} = 140 ft = 2.10 bar



PROJECT

6

Design of a New, 100,000-Metric-Tons-per-Year Cumene Production Facility

C.6.1 BACKGROUND

In the opinion of our marketing research department, the demand for phenol-derived plasticizers is on the rise. Therefore, we are investigating the possibility of a new, grass-roots phenol plant to handle the anticipated increase. Because phenol is made from cumene, a grassroots cumene plant would also be necessary. Given your experience in troubleshooting our existing cumene process, we would like you to study the economics of a new cumene plant. Specifically, we would like a complete preliminary design of a grass-roots, 100,000 metric ton/y cumene process using benzene and propylene.

We have a new, proprietary catalyst, and the kinetics are included in Table C.17. We would also like you to consider the economics of our continuing to use propylene with 5% propane impurity at $0.095/lb versus purer propylene feed. In preparing this preliminary design, you should assume that all steam made can be used elsewhere in the plant with the appropriate economic credit, that condensed steam can be returned as boiler feed water for the appropriate credit, and that fuel gas can be burned for credit at its LHV (lower heating value). Additional information is given in Table C.18.

C.6.2 ASSIGNMENT

Your assignment is to provide the following:

1. An optimized preliminary design of a plant to make cumene from benzene and propylene using the new catalyst
2. An economic evaluation of your optimized process, using the following information:
   - After-tax internal hurdle rate = 9% p.a.
   - Depreciation = MACRS (6-year schedule; see Chapter 9)
   - Marginal taxation rate = 35%

Table C.17 Reaction Kinetics for Cumene Reactions (Unit 800)

The kinetics for the reactions are as follows:

$$\underset{propylene}{C_3H_6} + \underset{benzene}{C_6H_6} \xrightarrow{k_1} \underset{cumene}{C_9H_{12}}$$

$$r_1 = k_1 c_p c_b \quad \text{mole/g cat sec}$$

$$k_1 = 3.5 \times 10^4 \exp\left(\frac{-24.90}{RT}\right)$$

$$\underset{propylene}{C_3H_6} + \underset{cumene}{C_9H_{12}} \xrightarrow{k_2} \underset{p\text{-diisopropyl benzene}}{C_{12}H_{18}}$$

$$r_2 = k_2 c_p c_c \quad \text{mole/g cat sec}$$

$$k_2 = 2.9 \times 10^6 \exp\left(\frac{-35.08}{RT}\right)$$

where the units of the activation energy are kcal/mol, the units of concentration are mol/l, and the temperature is in Kelvin.

For a shell-and-tube packed bed, the recommended configuration, the following data may be assumed:

- Catalyst particle diameter $d_p = 3$ mm
- Catalyst particle density $\rho_{cat} = 1600$ kg/m^3
- Void fraction $\varepsilon = 0.50$
- Heat transfer coefficient from packed bed to tube wall $h = 60$ W/m^2°C
- Use standard tube sheet layouts as for a heat exchanger
- If tube diameter is larger than in tube sheet layouts, assume that tube cross-sectional area is 1/3 of shell cross-sectional area

- Construction period = 2 years
- Project plant life = 10 years after start-up

Specifically, you are to prepare the following by . . . (four weeks from now):

1. A written report detailing your design and profitability evaluation of the new process
2. A clear, complete, labeled process flow diagram of your optimized process including all equipment and the location of all major control loops
3. A clear stream flow table including T, P, total flowrate in kg/h and kmol/h, component flowrate in kmol/h, and phase for each process stream
4. A list of new equipment to be purchased, including size, cost, and materials of construction
5. An evaluation of the annual operating cost for the plant

Table C.18 Additional Information (Unit 800)

Cost of Manufacture

In order to estimate the cost of manufacture (not including depreciation), COM_d, you should use the following equation:

$$COM_d = 0.180\ FCI + 2.73\ C_{OL} + 1.23\ (C_{UT} + C_{WT} + C_{RM}) \tag{8.2}$$

The current MACRS method for depreciation should be used in your calculations (see Chapter 9).

Hints for Process Simulator

The CHEMCAD process simulator was used to generate the flow table given in Project 5. The hints given here are specifically directed to CHEMCAD users but should also be applicable for other process simulators.

Use SRK (Soave-Redlich-Kwong) thermodynamics package for VLE and enthalpy calculations for all the equipment in the process.

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger. Actual equipment may include several zones, so costing should be based on the actual equipment specifications.

For the reactor, you may use an isothermal reactor to estimate the volume of catalyst and heat-exchange area. For more accurate results, the temperature profile in the reactor should be modeled by completing a differential heat and material balance on the reactor.

For the distillation columns, you should use the Shortcut method (SHOR) to get estimates for the rigorous distillation simulation (TOWR or SCDS). The Shortcut method may be used until an optimum case is near. It is then expected that everyone will obtain a final design using rigorous simulation of the columns.

When simulating a process using "fake" streams and equipment, it is absolutely necessary that the process flow diagram you present not include any "fake" streams and equipment. It must represent the actual process.

6. An analysis of the after-tax NPV (10 years, 9%), and the discounted cash flow rate of return on investment (DCFROR) for your recommended process
7. A legible, organized set of calculations justifying your recommendations, including any assumptions made

C.6.3 REPORT FORMAT

This report should be in the standard design report format, consistent with the guidelines given in Chapter 29 (in this CD). It should include an abstract, results, discussion, conclusions, recommendations, and an appendix with calculations.