

Major No. 1 – Design Problems for the Acetone Production Facility

September 18, 1998

Background

You have recently joined a Design and Construction Company called FlawlessDesignCo. This company designs and supervises the construction of new chemical plants. Eighteen months ago, the company won a contract to design and build a 15,000 tonne/yr facility to produce 99.9 mol% pure acetone via the catalytic dehydrogenation of isopropanol. The design of the facility was completed three months ago, and the equipment specifications have been sent to vendors who are currently completing the construction of the equipment. The latest check showed that the construction of individual equipment is approximately 90% complete, and the schedule for the delivery of all the equipment to the site has been set.

Currently, FlawlessDesignCo is in a state of panic! Last week, a manager reviewed the design one last time, and she found that the design capacity specified in the original contract stated that the production capacity of the plant should be 15,000 tonne/yr. However, she also noted that the plant was to serve a dual purpose, and that some other solvents were to be produced during periods of low acetone demand. The contract states that the plant should be able to produce this amount of acetone (15,000 tonne) over a 6000 hr period. This information was not included in the engineering package and the plant was designed based on a standard operating year of approximately 8000 hr! This means that we have designed and ordered equipment for a process that is 25% undersized, i.e., we must scale-up the current design by 33%! Our client, in addition to suggesting that we change the name of our company, has told us that they will hold us to the contract. This means that they expect the plant to be commissioned at the design rate specified in the contract. Any additional costs incurred in order to correct this problem will be borne solely by FlawlessDesignCo.

Fortunately, we are well ahead of schedule and we have three months or so to “fix” the problem. You have been chosen as part of a two-person task force to evaluate the situation quickly from a process point of view. Clearly, a completely new design can be carried out and new equipment ordered. However, this will amount to millions of dollars of loss for our company. What you have been asked to do is to evaluate the existing design and make recommendations as to the additional equipment that will be required in order for the plant to produce the contractual amount of acetone. The object is to minimize the cost for this additional equipment, i.e., key is to make the best use of equipment that has already been ordered and built.

For the purpose of this assignment, you should consider only the reactor feed, the reactor, and crude product separation sections, as shown in Figure 1. A summary of the designed and ordered equipment is given in Table 1. The streams leaving the process unit are Streams 7 and 9. Stream 7 contains the non-condensable gases and is burned as a fuel supplement in the boiler plant (not shown). Stream 9 contains acetone, water, and unreacted isopropyl alcohol. This is sent to the

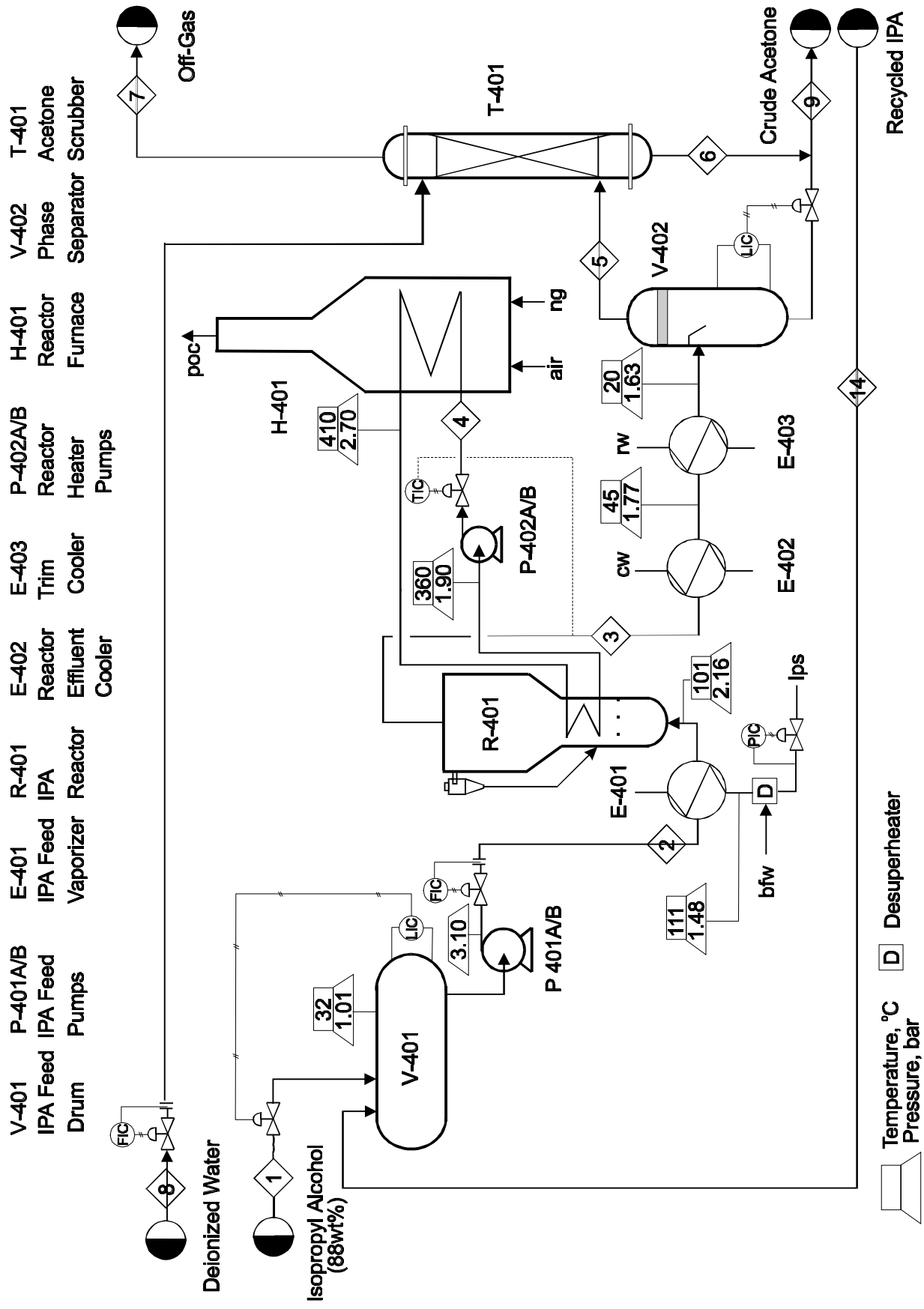


Figure 1: Preliminary Process Flow Diagram for the Production of Acetone

Table 1: Preliminary Equipment Summary Table for Acetone Process

Equipment	P-401 A/B	P-402 A/B	V-401	V-402
MOC	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Power (shaft) (kW)	0.43	1.58	-	-
Efficiency	40%	50%	-	-
Type/Drive	Centrifugal/ Electric	Centrifugal/ Electric	-	-
Op. Temperature (°C)	32	360	32	20
Pressure In (bar)	1.25	1.90	-	-
Pressure Out (bar)	3.10	3.30	-	-
Diameter (m)	-	-	0.80	0.75
Height/Length (m)	-	-	2.40	2.25
Orientation	-	-	Horizontal	Vertical
Internals	-	-	-	SS Demister
Op. Pressure (bar)	-	-	1.0	1.63
Maximum allowable operating pressure (bar)			3.0	3.2

Table 1: Preliminary Equipment Summary Table for Acetone Process (cont'd)

Equipment	T-401	H-401	R-401
MOC	Carbon Steel	Carbon Steel	Carbon Steel
Diameter (m)	0.32	-	Width = 4.57 m
Height/Length (m)	3.20	-	Depth = 6.10 m Height = 5 m
Orientation	Vertical	-	Vertical
Internals	2.5 m of Packing (1" Ceramic Rashig Rings)	-	Fluidized Bed containing 7.5 m ³ of catalyst + 7.8 m ³ of inert particles. Heat transfer area = 188 m ²
Op. Pressure (bar)	1.6	3.0 tube side	2.16 in bed 2.70 in tubes
Maximum allowable operating pressure (bar)	3.2	4.0	3.2 in bed 4.0 in tubes
Type	-	Fired Heater	-
Design Duty (MJ/h)	-	3436	3436
Maximum Duty (MJ/h)	-	3800	-
Area Radiant (m ²)	-	13.0	-
Area Convective (m ²)	-	37.0	-

Table 1: Preliminary Equipment Summary Table for Acetone Process (cont'd)

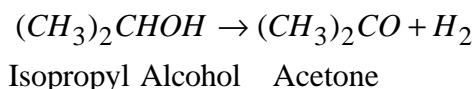
Equipment	E-401	E-402	E-403
Type	Float. Head Vaporizer	Float. Head Partial Cond.	Float. Head Partial Cond.
Duty (MJ/h)	2,850	3,251	568
Design Area (m ²)	79.2	73.6	8.8
Area as Built (m ²)	83.2	77.3	9.2
Shell Side			
Op. Temp (°C)	101	350	45
Op. Pressure (bar)	2.3	1.91	1.77
Maximum allowable operating pressure (bar)	3.2	3.2	3.2
Phase	Boiling Liq.	Cond. Vapor	Cond. Vapor
MOC	Carbon Steel	Carbon Steel	Carbon Steel
Tube Side			
Op. Temp (°C)	111	40	15
Op. Pressure (bar)	1.48	3.0	3.0
Maximum allowable operating pressure (bar)	6.0	5.0	5.0
Phase	Cond. Steam	L cooling water	L refrig. water
MOC	Carbon Steel	Carbon Steel	Carbon Steel

separations section of Unit 400 where specification acetone (99.9 mol%) is produced and the unused isopropyl alcohol is concentrated and returned to the feed tank, V-401, as Stream 14. For now, you may assume that the separations section can handle the increased flow of Stream 9. However, this is contingent on the pressure and temperature of Stream 9 remaining unchanged from the design conditions. The current design conditions are shown in the attached Stream Summary Table, Table 2.

Process Background and Data

Process Notes

The prevalent process for the production of acetone is as a by-product of the manufacture of phenol. Benzene is alkylated to cumene which is further oxidized to cumene hydroperoxide and finally cleaved to yield phenol and acetone. However, the process used here uses isopropyl alcohol (IPA) as the raw material. This is a viable commercial alternative, and a few plants operate using this process. The primary advantage of this process is that the acetone produced is free from trace aromatic compounds, particularly benzene. For this reason, acetone produced from IPA is favored by the pharmaceutical industry due to the very tight restrictions placed on solvents by the Food and Drug Administration (FDA). The reaction to produce acetone from IPA is given below:



The reaction conditions are typically around 2 bar and 350°C. At these conditions, single-pass conversions of 85-92 % are possible. The design conditions used here are given in Tables 1 and 2, and a single-pass conversion of 90% is used.

Process Description

The process designed by our company is shown in Figure 1. An azeotropic mixture of isopropyl alcohol and water (88 wt% IPA), Stream 1, is fed into a surge vessel (V-401) where it is mixed with the recycled unreacted IPA/water mixture, Stream 14. This material is then pumped to heat exchanger E-401, where it is vaporized prior to entering the reactor. Heat is provided for the endothermic reaction using a circulating stream of molten salt, Stream 4. The reactor effluent, Stream 3, containing acetone, hydrogen, water, and unreacted IPA, is cooled in two exchangers, E-402 and E-403, prior to entering the phase separator (V-402). The vapor leaving the separator, Stream 5, is scrubbed with water to recover additional acetone, and then this liquid, Stream 6, is combined with the liquid from the separator and sent to the separations section as Stream 9. The non-condensable gases leaving the Acetone Scrubber, T-401, are sent off-site to the boiler plant where they are burned to recover their fuel value. Stream 9 is sent for further processing to two towers. These towers are used to separate the acetone product (99.9 mole %) and to remove the excess water from the unused IPA. The unused reactant, Stream 14, is then recycled back to the front end of the process as a near azeotropic mixture. The purification section of the process is not shown in Figure 1 and you should not consider it further in your analysis.

Table 2: Flow Table for Acetone Process in Figure 1 (based on 8000 h/yr)

Stream No.	1	2	3	4	5	6
Temperature (°C)	25	32	350	360	20	27
Pressure (bar)	1.01	2.30	1.91	3.0	1.60	1.60
Vapor Fraction	0.0	0.0	1.0	0.0	1.0	0.0
Mass Flow (tonne/h)	2.40	2.67	2.67	35.1	0.34	0.46
Mole Flow (kmol/h)	51.96	57.84	92.63	-	39.76	20.94
Component Mole Flow (kmol/h)				Molten Salt		
Hydrogen	-	-	34.77	-	34.77	0.00
Acetone	-	0.16	34.94	-	4.38	1.71
Isopropyl Alcohol	34.82	38.64	3.87	-	0.16	0.14
Water	17.14	19.04	19.05	-	0.45	19.09

Stream No.	7	8	9	14
Temperature (°C)	34	25	22	83
Pressure (bar)	1.50	2.0	1.6	1.2
Vapor Fraction	1.0	0.0	0.0	0.0
Mass Flow (tonne/h)	0.24	0.36	2.79	0.27
Mole Flow (kmol/h)	38.82	20.00	73.81	5.88
Component Mole Flow (kmol/h)				
Hydrogen	34.77	-	0.00	-
Acetone	2.67	-	32.27	0.16
Isopropyl Alcohol	0.02	-	3.85	3.82
Water	1.36	20.00	37.69	1.90

Utility	lps	cw	rw
Equipment	E-401	E-402	E-403
Temperature In (°C)	111	30	5
Temperature Out (°C)	111	40	15
Flow (tonne/h)	1.28	77.80	13.60
Low pressure steam is supplied at 6 bar (sat) from header			

Reaction Kinetics

The reaction to form acetone from isopropyl alcohol (isopropanol) is endothermic with a standard heat of reaction of 62.9 kJ/mol. The reaction is kinetically controlled and occurs in the vapor phase over a catalyst. The reaction kinetics for this reaction are first order with respect to the concentration of alcohol and can be estimated from the following equation:

$$-r_{IPA} = k_0 \exp\left[\frac{-E_a}{RT}\right] C_{IPA} \quad \frac{\text{kmol}}{\text{m}^3 \text{bulk catalyst s}}$$

with $E_a = 72.38 \text{ MJ/kmol}$, $k_0 = 3.51 \times 10^5 \frac{\text{m}^3 \text{gas}}{\text{m}^3 \text{bulk catalyst s}}$, C_{IPA} has units of $\left[\frac{\text{kmol}}{\text{m}^3 \text{gas}} \right]$

Several side reactions occur to a small extent. Thus, trace quantities of propylene, diisopropyl ether, acetaldehyde, and other hydrocarbons and oxides of carbon are also formed. The non-condensables are removed with the hydrogen while the aldehydes and ethers can be removed with acid washing or adsorption. These side reactions are not accounted for in the preliminary design shown in Figure 1. For now, you should not consider these side reactions further.

The reactor design used in the current process consists of a fluidized bed containing solid catalyst and inert solids. The endothermic heat of reaction is supplied by a circulating flow of molten salt heat transfer fluid that passes through heat transfer tubes immersed in the bed. This molten salt provides the heat required to maintain the fluidized bed at 350°C, and the molten salt is circulated through a fired heater where its temperature is raised to 410°C. This reactor configuration can be accurately modeled as an isothermal plug flow reactor. Due to selectivity considerations, the maximum temperature of the fluidized bed should not exceed 375°C, and the maximum single pass conversion should not exceed 95%. If single-pass conversions other than 90% are used, then the compositions of Streams 9, 7, and 14 will change. You may assume that the recovery of unused alcohol in the separations section is the same as in the base case.

Properties of the solid catalyst are as follows:

solid density, $\rho_s = 2500 \text{ kg/m}^3$, bulk density, $\rho_{\text{bulk}} = 1200 \text{ kg/m}^3$, particle size, $d_p = 100 \text{ mm}$

Inert filler particles have the same properties as the catalyst.

Vapor-Liquid Equilibrium

The VLE used to simulate the Acetone Scrubber, T-401, was derived from the UNIQUAC thermodynamics package using a latent heat enthalpy model. The equilibrium curve is given on page 22 of this assignment.

Capital Cost Estimations

In order to estimate the capital investments for new equipment, you should use the CapCost program contained on the CD in the back of the book. Beware! There is a bug in the program

which manifests itself when importing and editing previously saved files. When importing files, do not use the edit command, but rather delete the equipment that you wish to change and reenter the data for it.

Assignment

Your assignment is to prepare a written and oral report summarizing your findings and recommendations. The written report is due by 9:00 am, Monday September 27, 1998. The oral reports will follow during the week of September 27 – October 1. You should read carefully the guidelines for written and oral reports and Chapters 22 and 23 in the book “Analysis, Synthesis, and Design of Chemical Processes.” These chapters cover the required guidelines for written and oral presentations. The written report should not exceed 7 pages of double-spaced text, plus figures and tables. All relevant calculations should be included in a well-indexed appendix. These calculations should be neat and legible but may be hand written. The form of the report should be an executive summary (same organization as a long report but without section headings), which clearly and succinctly presents your major findings, explanations, conclusions, and recommendations. The following information must appear in the main body of the report:

- a. A computer generated process flow diagram (PFD) showing the configuration of equipment for your recommended case.
- b. A flow summary table showing the amounts and conditions of the streams shown in the PFD.
- c. A list of all new equipment with purchase and bare-module costs.
- d. Design details of all the new equipment.
- e. A copy of the confidentiality statement, signed by both team members. This should be the very last page of the written report.

Please provide the written report in a 3-ring, spiral or riveted binder (not oversized).

As explained previously, one person will be asked to present the formal oral report while the other person will be required to take the lead role in answering questions on the work. The formal oral presentation should take between 10 and 15 minutes and the question and answer session should take between 30 and 40 minutes. The choice of who does what will be made randomly at the beginning of the oral session. This means that both team members must prepare for both tasks. You must bring a hard copy of your slides to leave behind after the oral presentation.

Additional Technical Data

To help you in your analysis, a set of design calculations for the equipment in Figure 1 has been appended to this assignment. In addition to this data, you may assume/use the following information:

1. The cooling water and refrigerated water flows to E-402 and E-403, respectively, may be increased by a maximum of 20% over the design conditions for long periods of operation.
2. All heat transfer coefficients given in the appendix are correct for the design flows.
3. Pump performance curves for P-401 and P-402 are given in Figures 2 and 3, respectively. These are the performance curves for the pumps to be delivered to the site.

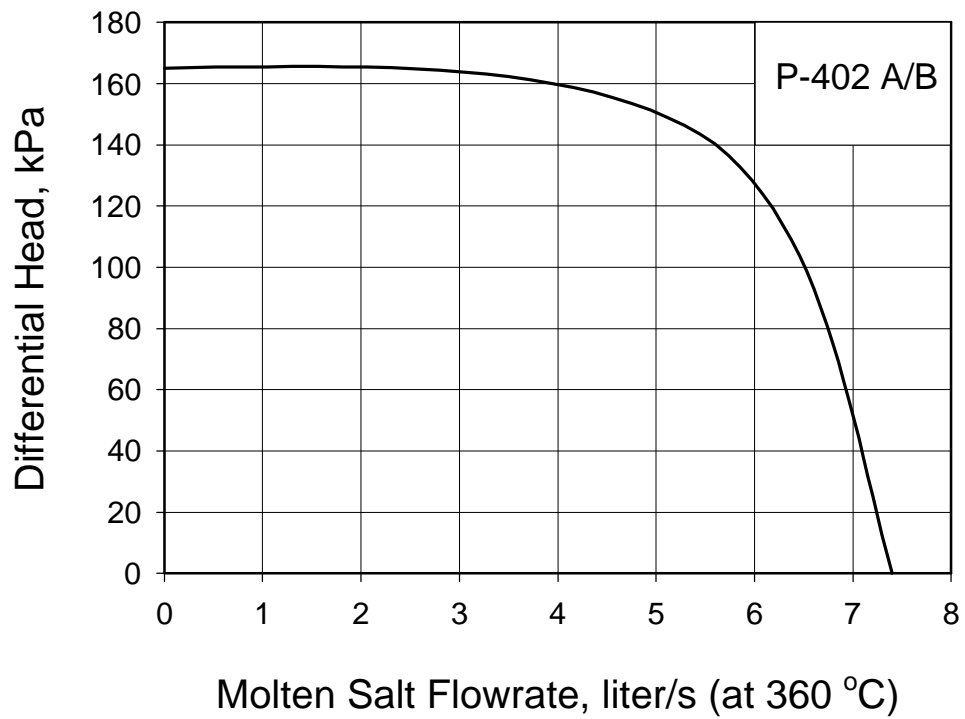
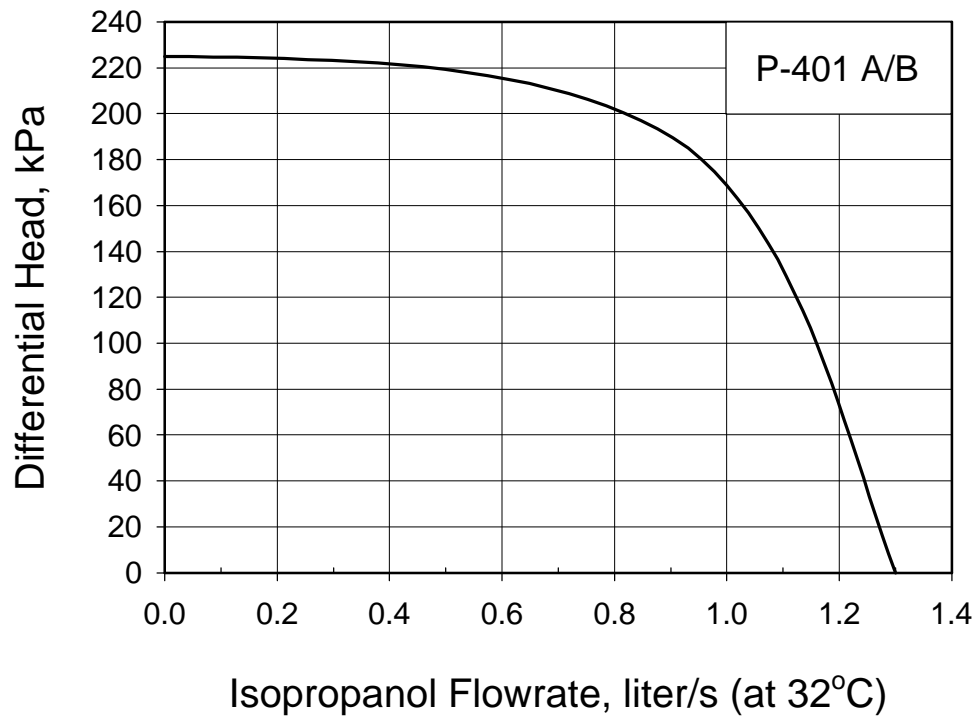


Figure 2: Pump Curves for P-401 A/B and P-402 A/B

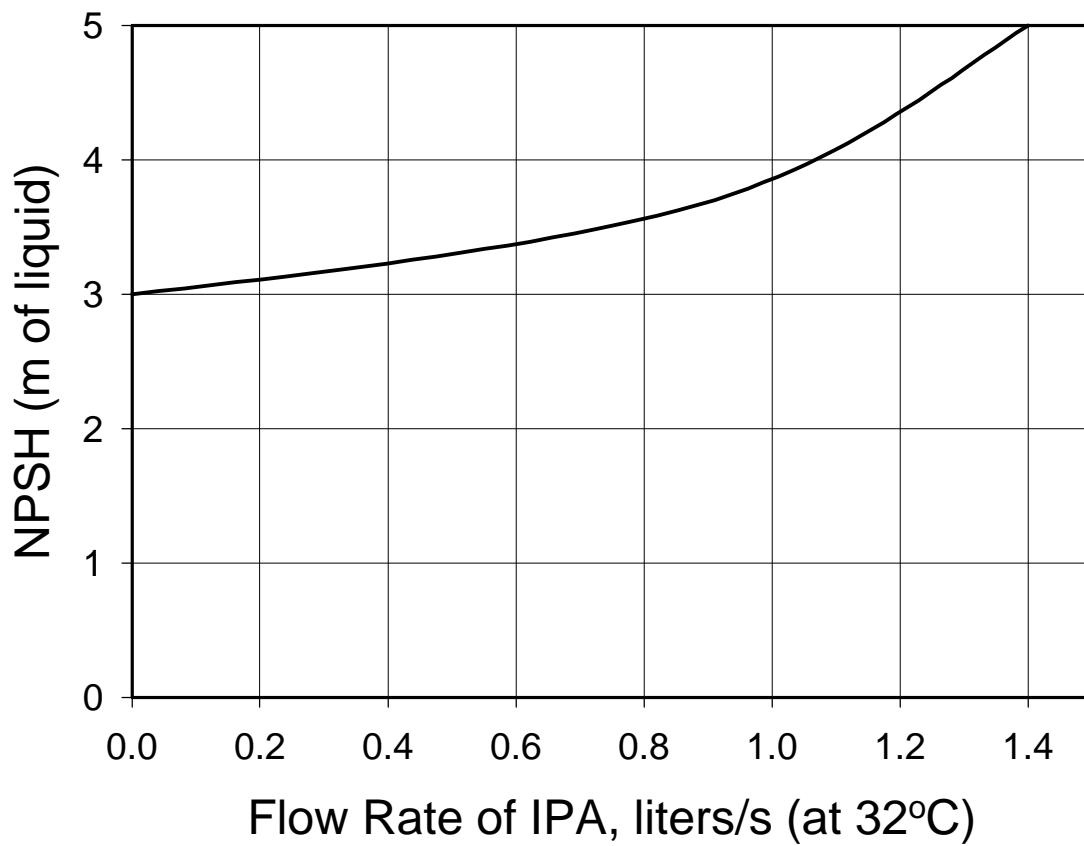
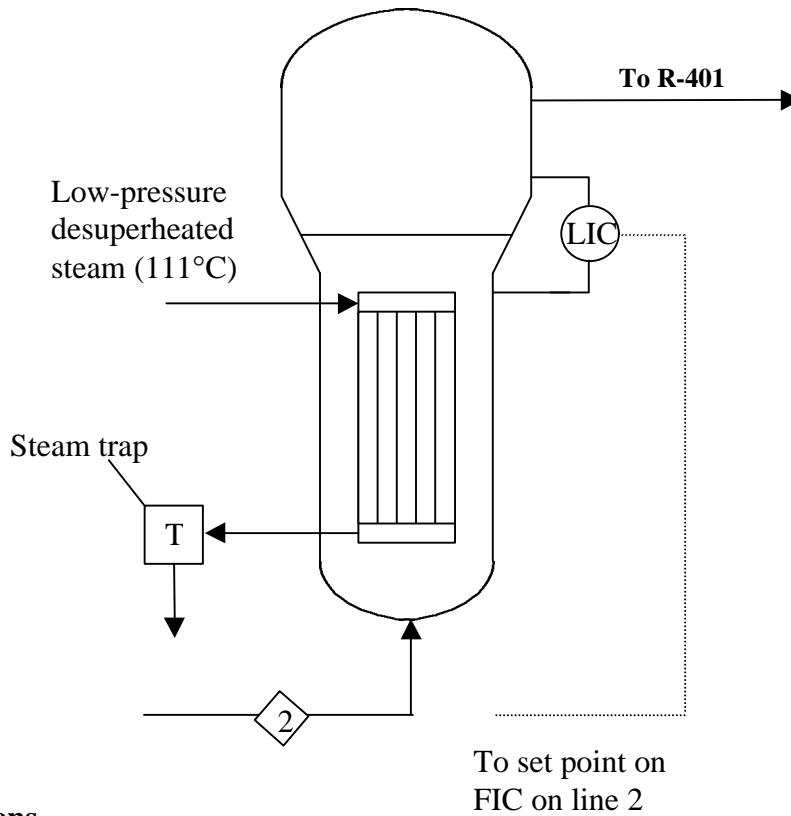


Figure 3: NPSH required by Pump, P-401 A/B, IPA Feed Pump

Appendix

Design Calculations

E-401 – Vertical Tube Vaporizer



Conditions

Vapor leaves E-401 at 2.16 bar and 101°C (saturated vapor). The shell side is assumed to be well mixed and at 101°C.

Heat Transfer Calculations

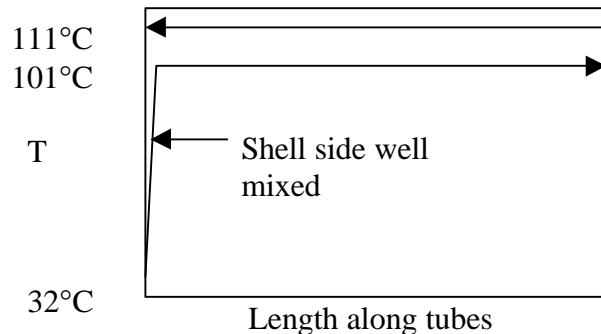
1. Regulate steam pressure to give a 10°C temperature driving force $\Rightarrow T_{\text{sat}} = 111^\circ\text{C}$ which corresponds to a $P_{\text{sat}} = 1.48$ bar.
2. Heat Duty = 2850 MJ/h , $C_{p,L} = 2880$ J/kg°C
3. Limiting heat transfer resistance is on boiling organic side, $h_{\text{shell}} = 1000$ W/m²°C.

$$\therefore U \approx h_{\text{shell}} = 1000 \text{ W/m}^2\text{°C}$$

$$\Delta T_{\text{lm}} = \Delta T = 10^\circ\text{C}$$

$$A = Q/U \Delta T_{\text{lm}} (F=1)$$

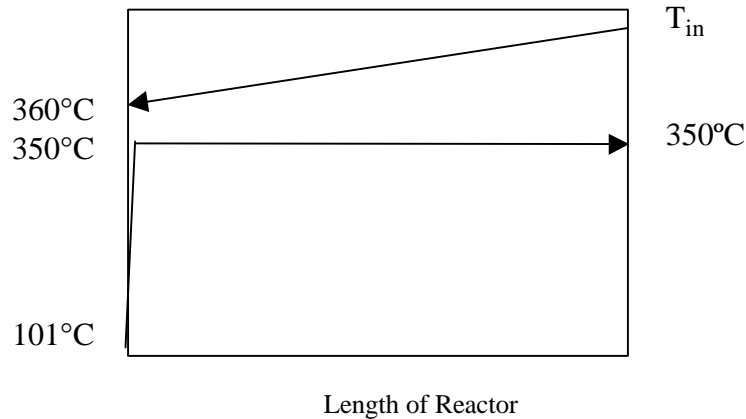
$$= 2850 \times 10^6 / 3600 / 1000 / 10 = 79.2 \text{ m}^2$$



Note: over the range of $\Delta T = 7$ to 25°C it is known that $h \propto \Delta T^{1/3}$ for boiling isopropanol.

Reactor R-401 – Heat Transfer Calculations

Assume that the fluidized bed is well mixed, thus the feed gas immediately heats to the reactor temperature of 350°C. The molten salt approach temperature is 10°C and therefore the molten salt temperature leaving the reactor is 360°C. The temperature vs. Q diagram is shown below:



$$Q=3436 \text{ MJ/h}$$

$$C_{p, \text{ gas}} = 1780 \text{ J/kg}^\circ\text{C} \text{ (inlet) and } 2500 \text{ J/kg}^\circ\text{C} \text{ (outlet)}$$

Use HiTec™ molten salt with the following average physical properties:

$$C_p = 1.72 \text{ kJ/kg K}, \rho = 1980 \text{ kg/m}^3, \mu = 2.1 \text{ cP},$$

maximum operating temperature = 1000°C

$$\text{Use a } \Delta T = 50^\circ\text{C} \text{ for the circulating salt } \therefore T_{\text{in}} = 410^\circ\text{C}$$

$$\Delta T_{\text{lm}} = (410-360)/\ln[(410-350)/(360-350)] = 27.9^\circ\text{C}$$

Energy balance on molten salt

$$Q=MC_p \Delta T \Rightarrow 3436 \times 10^6 = (M)(1720)(50)$$

$$M = 39,950 \text{ kg/h} = 11.10 \text{ kg/s}$$

$$\text{Vol flow of salt} = M/\rho = 11.10/1980 = 5.605 \times 10^{-3} \text{ m}^3/\text{s}$$

Evaluation of U

$$\text{Fluidized Bed to tube wall, } h_o = 200 \text{ W/m}^2\text{C}$$

[this will not change much with fluidization velocity in the range of 2 – 5 u_{mf}]

Inside heat transfer coefficient [molten salt to wall], $h_i = ?$

Assume that the velocity in the tubes is 2 ft/s = 0.61 m/s

Use ½" diameter tube 18 BWG with inside diameter = 0.01021 m

$$Re = (0.61)(0.01021)(1980)/(0.0021) = 5872$$

$$Nu = 0.023Re^{0.8}Pr^{0.33} = (.023)(5872)^{0.8}(1720 \times 0.0021/0.606)^{0.33} = 42.9$$

(actually Seider-Tate is only good for $Re > 10,000$ - check this later)

$$h_i = Nu[k/d] = (42.9)(0.606)/(0.01021) = 2546 \text{ W/m}^2\text{C}$$

Below 500°C molten salt should not foul so $h_f =$ very large

$$\text{Overall heat transfer coefficient, } U_o = [d_o/(d_i h_i) + 1/h_o]^{-1} = [1.244/2546 + 1/200]^{-1} = 182 \text{ W/m}^2\text{°C}$$

$$\text{Heat transfer area, } A_o = Q/U_o \Delta T_{lm} = (3436 \times 10^6) / [(3600)(182)(27.9)] = 188 \text{ m}^2$$

Check tube arrangement and molten salt velocity

$$\text{External surface area of 20 ft tubes} = \pi d_o L = (3.142)(0.0127)(20)(0.3048) = 0.243 \text{ m}^2$$

$$\text{Number of tubes} = (188)/(0.243) = 773$$

Use 110 parallel sets of 7 tubes piped in series

$$\text{Cross sectional area (csa) for flow of molten salt} = (110)(3.142)(0.01021)^2/4 = 0.0090 \text{ m}^2$$

$$\text{Velocity of molten salt in tubes} = 5.605 \times 10^{-3} / 0.0090 = 0.622 \text{ m/s}$$

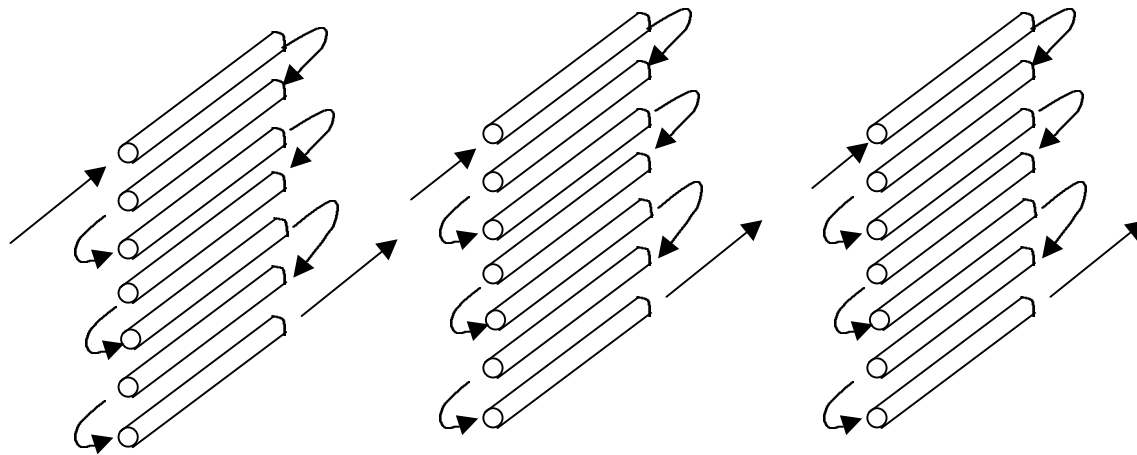
This gives $Re = 5988$ and $Nu = 43.6$ and $h_i = 2588$ and $U = 182 \text{ W/m}^2\text{°C}$ no change

For $Re < 10,000$ we should use correlation from Walas [1]:

$$Nu = 0.012 [Re^{0.87} - 280] Pr^{0.4} \left[1 - \left(\frac{d}{L} \right)^{2/3} \right]$$

This gives $Nu = 41.1$ and $h = 2438$, thus $U = 181 \text{ W/m}^2\text{°C}$ same as before.

Arrangement of tubes in Fluidized Bed



110 parallel banks of 7 tubes in Fluidized Bed Reactor, R-401

Height of Catalyst and Filler in Bed

Use a square tube pitch of 1.5 inches

Dimensions of tube bank are $110 \times 1.5/12$ by $7 \times 1.5/12$ by 20 ft = 13.75 by 0.875 by 20 ft

Assume bed width and depth of 15 by 20 ft respectively

Volume of solids to just cover the tubes, assuming bottom row of tubes is 6" from distributor plate and 6" of solids above tube bank = V_{sol}

$$\begin{aligned} V_{sol} &= (15)(20)(1+0.875) - \text{volume occupied by tubes} \\ &= 562.5 - (770)(20)(\pi)(0.5)^2/(4 \times 144) = 541.5 \text{ ft}^2 = 15.3 \text{ m}^3 \end{aligned}$$

Calculate the amount of catalyst required for 90% conversion

For a first order, isothermal, irreversible reaction at constant pressure we have the following expression for the conversion of component A, X_A :

$$kt = (1 + e_A) \ln \frac{1}{1 - X_A} - e_A X_A$$

From the kinetics expression, at a reactor temperature of 350°C, we have:

$$k = k_o \exp\left[\frac{-E_a}{RT}\right] = 3.51 \times 10^5 \exp\left[\frac{-72,380}{(8.314)(273 + 350)}\right] = 0.2996 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bulk catalyt} \cdot \text{s}}$$

$$\begin{aligned} \epsilon_A &= \frac{\text{number of moles if completely reacted} - \text{number of moles initially}}{\text{number of moles initially}} \\ &= \frac{(96.48 - 57.84)}{(57.84)} = 0.668 \end{aligned}$$

using above values and 90% conversion we get:

$$\begin{aligned} kt &= (1 + 0.668) \ln \frac{1}{1 - 0.9} - (0.668)(0.9) = 3.2395 \\ t &= (3.2395)/(0.2996) = 10.813 \frac{\text{m}^3 \text{ bulk catalyst s}}{\text{m}^3 \text{ gas}} \end{aligned}$$

$$V_{catalyst} = \dot{v}_{gas} t$$

now the volumetric flow rate of gas, $v_{gas} = 0.696 \text{ m}^3/\text{s}$

$$\therefore V_{catalyst} = (0.696)(10.813) = 7.5 \text{ m}^3 \text{ bulk catalyst}$$

Amount of catalyst required is 7.5 m^3 , therefore we must add 7.8 m^3 of inert filler to give a total of 15.3 m^3 of bed solids. This will give a slumped bed height approximately 6" above the top of the tube bank.

Check minimum fluidizing velocity

Cross sectional area (csa) of bed = $300 \text{ ft}^2 = 27.9 \text{ m}^2$

properties of gas flowing through fluidized bed:

$\rho = 1.067 \text{ kg/m}^3$, $\mu = 18.2 \times 10^{-6} \text{ kg/m.s}$

flow of gas = 2670 kg/h

vol flow of gas = $(2670)/[(1.067)(3600)] = 0.696 \text{ m}^3/\text{s}$

superficial gas velocity, $u = (0.696)/(27.9) = 0.0250 \text{ m/s}$

catalyst particles are approximately 100 mm in diameter, and have a density of 2500 kg/m^3 and bulk density of 1200 kg/m^3 . Calculate minimum fluidizing velocity using the correlation due to Wen and Yu [2]

$$\text{Re}_{p,mf} = [33.7^2 + 0.0408\text{Ar}]^{1/2} - 33.7 \quad \text{where } \text{Ar} = d_p^3 \rho_g (\rho_s - \rho_g) g / \mu^2$$

$$\text{Ar} = (10^{-4})^3 (1.067)(2500 - 1.067)(9.81) / (18.2 \times 10^{-6})^2 = 78.97$$

$$\text{Re}_{p,mf} = [33.7^2 + 0.0408(78.97)]^{1/2} - 33.7 = 0.0478$$

$$u_{mf} = (0.0478)(18.2 \times 10^{-6}) / [(1.067)(10^{-4})] = 0.00815 \text{ m/s}$$

$$u/u_{mf} = 0.0250/0.00815 = 3.06 \Rightarrow \text{O.K.}$$

Cyclones can handle solids and gas in the range $1 < u/u_{mf} < 5$

Pressure Drop Across Fluidized Bed

Height of solids in fluidized bed = $1.875 \text{ ft} = 0.57 \text{ m}$

$$\Delta P_{bed} = h \rho_{bulk} g = (0.57)(1200)(9.81) = 6727 \text{ Pa} = 0.067 \text{ bar}$$

Distributor loss = $0.6 \Delta P_{bed} = 0.040 \text{ bar}$

Internal cyclone losses = 0.14 bar

(The design of the cyclones has been based on a maximum superficial gas velocity of $5u_{mf}$)

$$\text{Total loss across bed} = 0.067 + 0.040 + 0.14 \approx 0.25 \text{ bar}$$

Use a reactor height of 5.0 m to accommodate solids bed, plenum, freeboard, and cyclones.

Pressure Drop of Molten Salt through Heat Transfer Tubes

Re for molten salt flow = 5988

Roughness of drawn tubes, $e = 0.0015 \text{ mm}$

$$e/d = 0.0015/10.21 = 0.00015$$

$$f = 0.0087$$

$$d = 0.01021 \text{ m}$$

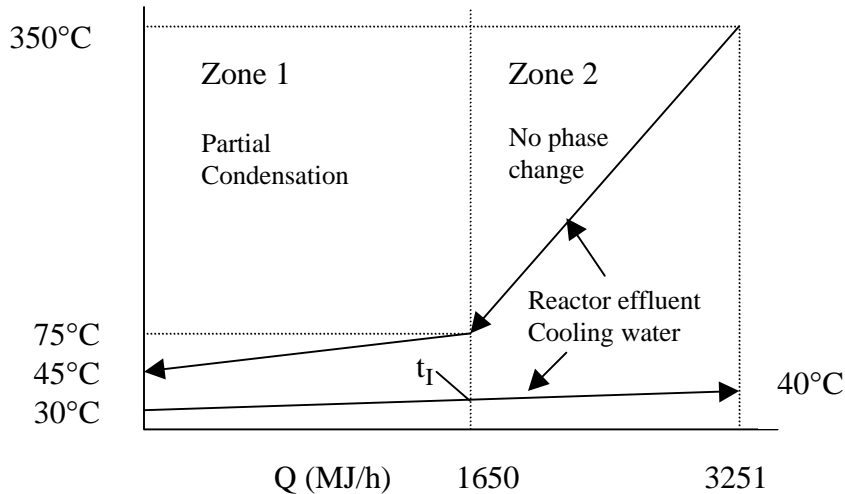
$$\rho = 1980 \text{ kg/m}^3$$

$$\begin{aligned} L_{eq} &= \text{length of tube} + \text{equivalent length of } 12\text{-}90^\circ \text{ bends} = (7)(20)(.3048) + (12)(30d) \\ &= 46.3 \text{ m} \end{aligned}$$

$$\Delta P_f = 2pfL_{eq}u^2/d = (2)(1980)(0.0087)(46.3)(0.622)^2/(0.01021) = 60443 \text{ Pa} = 60.4 \text{ kPa}$$

E-402 Reactor Effluent Cooler - Partial Condenser

$$Q = 3251 \text{ MJ/h}$$



Energy Balance on Cooling Water

$$mc_p\Delta T = (3251 \times 10^6) / (3600) = 903 \text{ kW}$$

$$m = (903000) / [(4180)(10)] = 21.6 \text{ kg/s}$$

$$\text{intermediate temperature, } t_1 \Rightarrow (40 - 30) / 3251 = (t_1 - 30) / 1650 \Rightarrow t_1 = 35.1^\circ\text{C}$$

Zoned Analysis

Zone 1

$$Q_1 = 1650 \text{ MJ/h} = 458.3 \text{ kW}$$

$$\Delta T_{\text{lm},1} = [(75 - 35.1) - (45 - 30)] / \ln[(75 - 35.1) / (45 - 30)] = 25.5^\circ\text{C}$$

U_1 partial condensation from an incompressible gas

$$h_{\text{cw}} = 2000 \text{ W/m}^2\text{C}$$

$$h_{\text{pcond}} = 1710 \text{ W/m}^2\text{C}$$

$$U_1 \approx [1.244 / 2000 + 1 / 1710]^{-1} = 829 \text{ W/m}^2\text{C}$$

$$A_1 = (458,300) / [(829)(25.5)] = 21.7 \text{ m}^2$$

Zone 2

$$Q_2 = (3251 - 1650) = 1601 \text{ MJ/h} = 444.7 \text{ kW}$$

$$\Delta T_2 = [(350 - 40) - (75 - 35.1)] / \ln[(350 - 40) / (75 - 35.1)] = 131.7^\circ\text{C}$$

$$h_{\text{cw}} = 2000 \text{ W/m}^2\text{C}$$

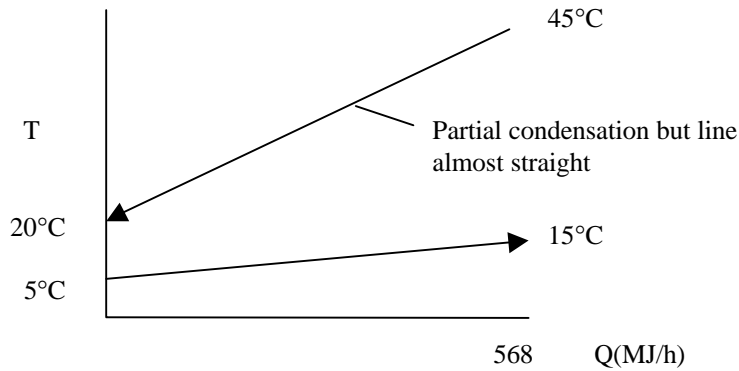
$$h_{\text{gas}} = 68 \text{ W/m}^2\text{C}$$

$$U_2 = [1 / 68 + 1.244 / 2000]^{-1} = 65 \text{ W/m}^2\text{C}$$

$$A_2 = (444700) / [(65)(131.7)] = 51.9 \text{ m}^2$$

$$\text{Total area} = 51.9 + 21.7 = 73.6 \text{ m}^2$$

E-403 Trim Cooler



$$Q = 568 \text{ MJ/h} = 157.8 \text{ kW}$$

$$\Delta T_{\text{lm}} = (30-15)/\ln(30/15) = 21.6^\circ\text{C}$$

$$U = 829 \text{ W/m}^2\text{C}$$

$$A = (157800)/[(829)(21.6)] = 8.8 \text{ m}^2$$

Pressure Drop for Molten Salt Loop (P-402 A/B located at ground level)

Pressure drops in loop	$\Delta P_{\text{reactor}} = 60.4 \text{ kPa}$
	$\Delta P_{\text{heater}} = 30.0 \text{ kPa}$
	$\Delta P_{\text{control valve}} = 30.0 \text{ kPa}$
	$\Delta P_{\text{piping}} = 19.9 \text{ kPa}$ (see below)
	Total pressure drop = 140.3 kPa

Loop consists of 200 equivalent feet of 3" sch 40 pipe. ID = 0.0779 m

Flow of molten salt = $5.605 \times 10^{-3} \text{ m}^3/\text{s}$

Velocity of molten salt in pipe = $(5.605 \times 10^{-3})/[\pi(0.0779)^2/4] = 1.18 \text{ m/s}$

$Re = (1.18)(1980)(0.0779)/(0.0021) = 8.7 \times 10^4$

Pipe roughness, $e = 0.0046 \text{ mm}$

$e/d = (0.0046)/(77.9) = 6 \times 10^{-5}$

$f = 0.0046$

$\Delta P_{\text{friction}} = 2f\rho L_{\text{eq}}u^2/d = (2)(0.0046)(1980)(61)(1.18)^2/(0.0779) = 19.9 \text{ kPa}$

Pump (P-601 A/B) must pump 5.6 liter/s of molten salt at 350°C at 140 kPa differential head.

Vapor pressure of molten salt at 350°C is <1kPa – cavitation is not a problem.

Pressure Drop for IPA Feed Pumps, P-401 A/B (located at ground level)

Feed pressure = 1.01 bar

Destination pressure (Stream 9 BL) = 1.6 bar

Height of liquid in V-401 = 12 ft above ground = 3.66 m

Height of Stream 9 = 10 ft above ground = 3.05 m

$\Delta P_{12} = 1.6 - 1.01 = 0.59$ bar

$\Delta h_{pg} = (3.05)(830)(9.81) - (3.66)(797)(9.81) = -3.78$ kPa = -0.038 bar

Design flowrate of IPA = 2670 kg/h = 0.7417 kg/s

Physical properties of IPA: $\rho = 797$ kg/m³, $\mu = 1.324$ kg/m.s, $P_{32^\circ\text{C}}^* = 0.12$ bar

$$\begin{aligned}\text{Design } \Delta P &= \Delta P_{\text{line}} + \Delta P_{\text{E-401}} + \Delta P_{\text{R-401}} + \Delta P_{\text{E-402}} + \Delta P_{\text{E-403}} + \Delta P_{\text{V-401}} + \Delta P_{\text{control valve}} \\ &= \Delta P_{\text{line}} + 0.14 + 0.25 + 0.14 + 0.14 + 0.03 + \Delta P_{\text{control valve}} \\ &= 0.70 \text{ bar} + \Delta P_{\text{line}} + \Delta P_{\text{control valve}}\end{aligned}$$

From piping isometrics we have liquid lines of 3" sch 40 (ID = 3.068") and vapor lines of 12" sch 40 (ID = 11.938")

Liquid velocity in Stream 2 = $(0.7417)/[(797)(3.142)(0.07792)^2/4] = 0.195$ m/s

Gas properties for Stream 3: $\rho = 1.0662$ kg/m³, $\mu = 18.18 \times 10^{-6}$ kg/m.s

Velocity in Stream 3 = $(2675)/[(3600)(1.0662)(3.142)(0.3032)^2/4] = 9.65$ m/s

With these low velocities we can ignore the frictional losses in the lines, $\therefore \Delta P_{\text{line}} = 0$

Use $\Delta P_{\text{control valve}} = 0.60$ bar

Total $\Delta P_{\text{friction}} = 0.7 + 0.0 + 0.6 = 1.3$ bar

$\Delta P_{\text{pump}} = 1.3 + 0.59 - 0.04 = 1.85$ bar = 185 kPa

design flow through pump = $(0.7417)/(797) = 9.31 \times 10^{-4}$ m³/s = 0.931 liter/s

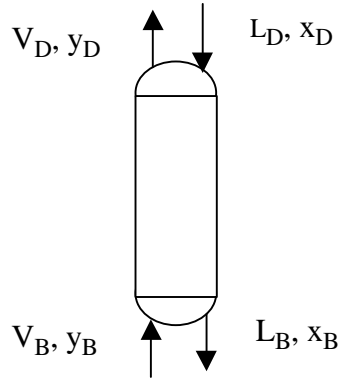
Pressure at pump discharge (pump outlet 2ft above ground level) = $P_{\text{discharge}}$

$$P_{\text{discharge}} = 1.01 + (12-2)(.3048)(797)(9.81)/(1 \times 10^5) + 1.85 = 3.10 \text{ bar}$$

Operation of Tower T-401

The equilibrium curve for acetone scrubber is shown in Figure A.1. Due to the non-linear equilibrium curve the maximum recovery of acetone is quite low. Typical operation of these absorbers in the past has given about 40% recovery (we use 39% here). Although, isopropanol is also absorbed, the limiting process is for the absorption of acetone. The total molar vapor and liquid flows do not change much and we may assume a straight operating line. The final design, giving the compositions in Table 2, was carried out on a process simulator. The following calculations were used to check this design.

Material Balance



The total flow of Stream 5 is 39.76 kmol/h ($V_B = 39.76$) containing 4.38 kmol/h of acetone ($y_B = 11.02$ mol%). If we recover 39% of this acetone in the water, the exit liquid, Stream 6 will contain 1.71 kmol/h of acetone. In addition, Stream 7 leaving T-401 will contain 2.67 kmol/h of acetone ($y_D = 6.88$ mol%). Assuming we use pure water in Stream 8 then $x_D = 0.0$. The limiting operating line is drawn in the top figure of Figure A.1 from the point (x_D, y_D) to just touch the equilibrium curve.

The slope of this line is

$$\left[\frac{L}{V} \right]_{\min} = \frac{(0.1065 - 0.0688)}{(0.090 - 0.0)} = 0.4189$$

$$L_{\min} = (0.4189)(39.76) = 16.7 \text{ kmol/h}$$

$$\Rightarrow \text{use } L = 20 \text{ kmol/h} \therefore (L/V) = 0.503$$

Operating line will pass through (x_D, y_D) and $(0.09, 0.114)$ this line is shown on bottom figure of Figure A.1. Stepping off stages we from graph we find that we need 5 theoretical stages.

Column Diameter and Loading Calculations

Limiting condition will be at the bottom of the column:

$$L_B = 20.94 \text{ kmol/h} = 460 \text{ kg/h (use physical properties of water)}$$

$$V_B = 39.76 \text{ kmol/h} = 342 \text{ kg/h } (\rho = 0.576 \text{ kg/h, } \mu = 9.36 \times 10^{-6} \text{ kg/m.s)}$$

Locate tower operation on Flooding Pressure Drop Curve (Treybal [3], page 195):

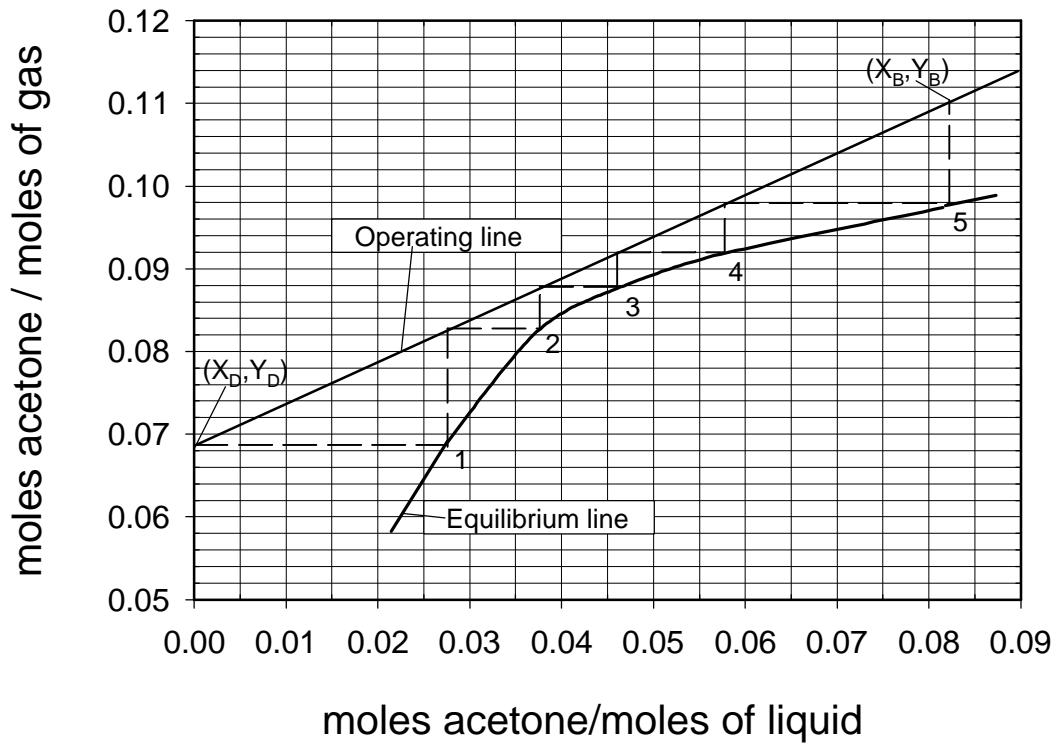
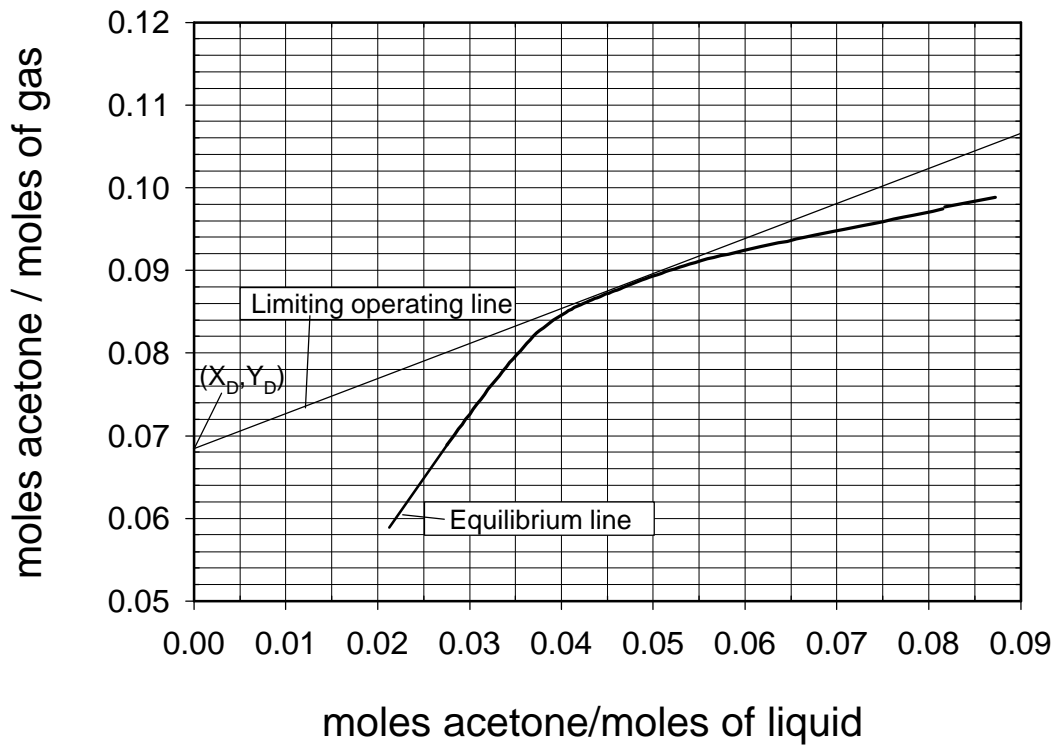


Figure A.1: Equilibrium Diagram for Acetone Scrubber, T-401

$$\frac{L'}{G'} \sqrt{\frac{\mathbf{r}_g}{\mathbf{r}_l - \mathbf{r}_g}} = \frac{460}{342} \sqrt{\frac{0.576}{1000 - 0.576}} = 0.032$$

Use 1" ceramic Rashig rings with a $C_f = 155$ (ref. [3], page 196)

From Standard Flooding and Pressure Drop curve we get a Flooding ordinate = 0.30

$$\therefore \frac{G'^2 C_f m_l^{0.1} J}{g_c (\mathbf{r}_l - \mathbf{r}_g) \mathbf{r}_g} = 0.30$$

The above relationship has dimensions and we must use the appropriate units, given below:

$$g_c = 4.18 \times 10^8$$

$$\mu_l = 1.0 \text{ cP}$$

$$G' = (342)(2.2048)/(\pi d_{col}^2/4) = 960.1 / d_{col}^2 \text{ lb/ft}^2\text{-h (where } d_{col} \text{ is in ft)}$$

$$J = 1.502$$

All densities are lb/ft³

$$\frac{(960.1/d_{col}^2)^2 (155)(1)^{0.1}(1.502)}{(4.18 \times 10^8)(62.4 - 0.03594)(0.03594)} = 0.30 \Rightarrow d_{col}^4 = 0.763 \Rightarrow d_{col} = 0.935 \text{ ft}$$

This is the minimum (flooding) diameter. Use a design with 80% of flooding

$$d_{col} = (0.935)/(0.8)^{1/2} = 1.045 \text{ ft} = 0.32 \text{ m}$$

With this value of column diameter the new ordinate value is 0.19 and pressure drop of packing is 1400 Pa/m of packing

HETP (height equivalent of a theoretical plate) = 0.5 m of packing/plate

$$\therefore \text{packed bed height} = (0.5)(5) = 2.5 \text{ m}$$

For operation in range of 40 – 90% of flooding 1" Rashig rings give almost constant HETP

$$\text{Pressure drop across packing} = (2.5)(1400) = 3.5 \text{ kPa}$$

Additional losses for inlet gas distributor = 6.5 kPa giving total column $\Delta P = 10 \text{ kPa} = 0.1 \text{ bar}$

References

1. Walas, S., M., *Chemical Process Equipment: Selection and Design*, Butterworth, Stoneham, MA, 1988, p. 190.
2. Wen, C.Y., and Y.H. Yu, *AIChE J.*, 12, 610 (1966).
3. Treybal, R.E., *Mass-Transfer Operations*, 3rd ed., McGraw-Hill, New York, 1980.