# NATIONAL UNIVERSITY OF ENGINEERING COLLEGE OF CHEMICAL AND TEXTILE ENGINEERING Professional School of Chemical Engineering

# PLANT DESIGN PI 525 A



# Design of an acetone production plant via catalytic dehydrogenation of isopropyl alcohol

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# DESIGN OF AN ACETONE PRODUCTION PLANT VIA CATHYTIC DEHYDROGENATION OF ISOPROPYL ALCOHOL

### 1. INTRODUCTION

In Process Engineering, a good design of the plant determines the future of the project in which it is intervened; and the high national and international competition for the market has the effectiveness of finding solutions to problems and nurturing a policy of taking initiatives, as well as incorporating innovation in technologies and processes. Therefore having a clear idea of methodology, creativity and knowledge is essential to guarantee what you want to get as a product or service. The present report shows the development of the design of a plant for the production of Acetone from Isopropyl Alcohol (IPA) by catalytic dehydrogenation which is intended to be adjustable to a capacity of 20 000 tonnes per year, optimum, controllable, with Low levels of pollutants and low production costs.

### Context

Acetone is widely used in industry, in the manufacture of Methyl Methacrylate (MMA), Methacrylic Acid, Methacrylates, Bisphenol A, among others, but it can also be used as:

- Solvent for most plastics and synthetic fibers.
- Ideal for thinning fiberglass resins.
- Cleaning of wool and fur garments.
- Clean fiberglass tools and dissolve epoxy resins.
- Cleaning of microcircuits and electronic parts.
- It is used as a volatile component in some paints and varnishes.
- It is useful in the preparation of metals before painting.

- Acetone is often used as a nail cleaner.

In the production of Acetone different methods are presented, of which three are outstanding: Cumene process, oxidation process of polypropylene and the process of dehydrogenation of Isopropyl alcohol. The Cumene process is the most common worldwide, but as a byproduct, is benzene (carcinogen) lowering the purity of Acetone and increasing production costs by separation. The oxidation of polypropylene has a low conversion of acetone and the purity of the reactants should be 99%. In the dehydrogenation of IPA, high purity Acetone is obtained, the IPA can be used in aqueous solution, and the conversion of acetone is high and has no substances, which are significantly hazardous to health. This process leaves us as the main product acetone from which its multiple uses were mentioned, and as secondary products: Hydrogen, widely used in the chemical industry: ammonia synthesis, refinery processes, coal treatment, among others. In this report, we opt for the dehydrogenation process of IPA, which offers great advantages and results with low production costs.

# 2. OBJECTIVES

# General objective:

Carry out the conceptual design of a 20,000 t / year production plant of 99.9%
molar acetone by catalytic dehydrogenation of isopropyl alcohol and check its
economic viability by finding the equilibrium price for the requested acetone
production capacity.

# **Specific objectives:**

• To structure the preliminary design of an acetone production plant, so that a careful and correct choice of the required operating equipment is made, specifying

the dimensions, materials, costs and operating capacity of each of them, in the proper sequence.

To look for the conditions of optimization of the productive process of the acetone
from isopropyl alcohol through the implementation of recycle streams, energy
integration and proper use of each equipment involved.

### 3. REVIEW OF THE TECHNOLOGY APPLIED TO THE CASE STUDY

There are different methods of obtaining acetone, among which one of the most used in the pharmaceutical industry is the process of catalytic dehydrogenation of isopropyl alcohol due to the high purity of the product; this process consists of a set of operations well known and used by process engineers.

# **Base Process Block Diagram**

The base case study deals with the production of acetone from isopropyl alcohol by the dehydrogenation reaction in the gas phase of the isopropyl alcohol in the presence of the catalyst, then undergoes cooling, condensation and purification (separation of impurities from the product - IPA, water) To obtain acetone with high purity (99.9%), with the said block diagram of the base process would be as follows:



In the block diagram shown, the main operations that make up the process are presented, which are justified by the following reasons:

- MIXING: The concentration of IPA in the feed is different from that recirculated from the top of the IPA distillation column, which contains small quantities of the product (acetone) that could not be separated in the acetone distillation column. For this reason, it is necessary to mix these two streams before entering the vaporizer, in order to homogenize the properties of the mixture.

The resulting mixture of IPA, water and a depreciable amount of acetone requires to be vaporized, since the catalytic dehydrogenation reaction is carried out in the gas phase in order to improve the contact between the catalyst and the reactant mixture.

- REACTOR: In order to carry out the reaction it is necessary to bring the feed mixture into contact with the catalyst, to supply the heat of reaction because it is endothermic, to feed the reactants and to withdraw the products in such a way as to favor the kinetics And selectivity. All these operations must be carried out in a reactor that allows the reactants to be converted into desired products.
- CONDENSER AND COOLING: The reactor outlet current is at high temperatures, for this reason it is necessary to cool this stream, to condense the IPA, acetone and water vapors in order to improve the separation of the liquid and gaseous phases in the Flash tab.

The reactor output stream is made up of product (acetone), water, unreacted isopropyl alcohol and hydrogen. In order to separate the desired product from the other components it is necessary to carry out several separation operations, which are:

- PHASE SEPARATOR: The formation of a liquid and gaseous phase after cooling allows using a flash separation, making it possible to separate all the hydrogen from the liquid phase because it has low (negligible) solubility. In the gas phase hydrogen and vapors of IPA, acetone and water will be in equilibrium with their liquids.

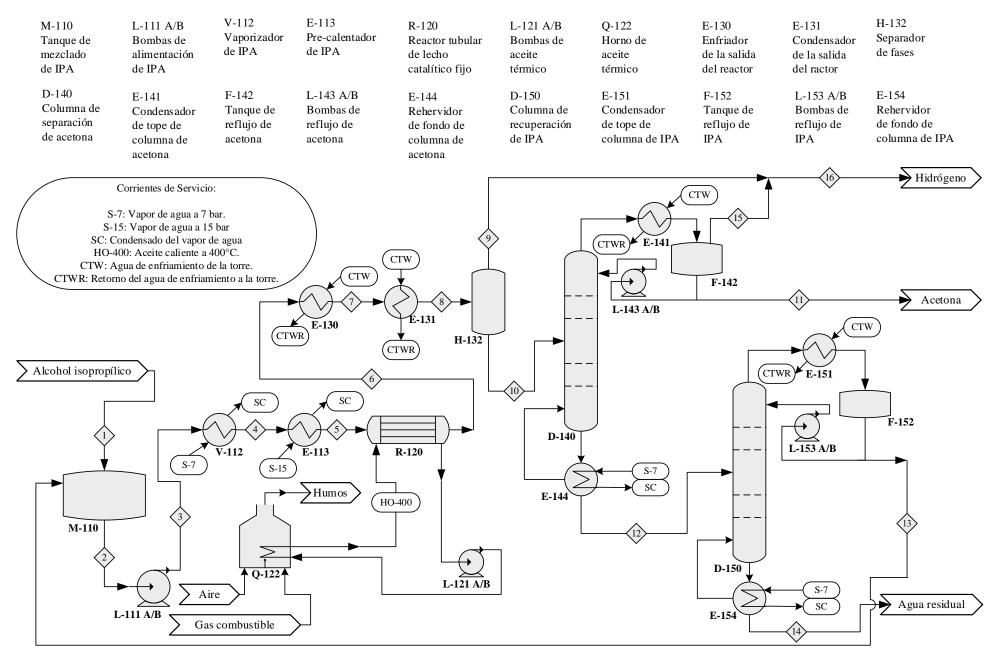
- ACETONE DISTILLATION: The liquid phase separator is fed to the distillation column, which is made up of water, IPA, acetone and traces of hydrogen. The separation in this operation is carried out taking advantage of the difference of volatilities of the 3 components, this allows to obtain the product (acetone) to the desired specification (99.9%) with a small amount of IPA at the top as the lighter components And a bottom stream consisting of IPA, water and a negligible amount of acetone to be separated in the next step.

- DISTILLATION OF IPA: The feed of this column is formed by the bottoms of the acetone distillation column. This operation allows obtaining a current of IPA and acetone (negligible) by the stop to be recirculated to the process and a bottom stream formed by IPA and water, whose concentration is limited by the capacity of the wastewater treatment system.

**Base Case Process Flow Diagram** 

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# **PFD:** Acetona vía deshidrogenación catalítica del alcohol isopropílico (IPA)



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# 4. BALANCE OF SUBJECT MATTERS

	Table: CURRENT MATERIAL BALANCE															
No. CURRENT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Mass flow (kg / h)	3280.27	3772.00	3772.00	3772.00	3772.00	3772.00	3772.00	3772.00	424.06	3347.94	2450.98	896.90	491.74	405.16	0.06	424.12
Molar flow (kmol / hr)	70.7809	81.5159	81.5159	81.5159	81.5159	128.9453	128.9453	128.9453	53.4962	75.4490	42.1986	33.2199	10.7350	22.485	0.0305	53.527
Temperature (° C)	25.0	33.5	33.5	117.0	180.00	387.65	92.2	32.0	32.0	32.0	45.8	107.0	96.45	130.0	45.8	38.9
Pressure (kPa)	99.8	99.8	400.0	380.0	360.0	340.0	320.0	300.0	300.0	300.0	280.0	300.0	250.0	260.0	99.8	99.8
Components (kmol / h)																
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	47.4294	47.4294	47.4294	47.3989	0.0305	0.0000	0.0000	0.0000	0.0000	0.0305	47.4294
Acetone	0.0000	2.1429	2.1429	2.1429	2.1429	49.5722	49.5722	49.5722	5.2729	44.2993	42.1564	2.1429	2.1429	0.0000	0.0000	5.2729
Isopropyl alcohol	47.6497	52.6993	52.6993	52.6993	52.6993	5.2699	5.2699	5.2699	0.1759	5.0940	0.0422	5.0518	5.0496	0.0022	0.0000	0.1759
Water	23.1312	26.6737	26.6737	26.6737	26.6737	26.6737	26.6737	26.6737	0.6485	26.0252	0.0000	26.0252	3.5426	22.4826	0.0000	0.6485

### 5. <u>DETERMINATION OF FIXED CAPITAL</u>

- For the determination of Fixed Capital Investment, it is necessary to make a good estimate of total equipment costs (Ce), since the other components of fixed capital (facilities, pipelines, services, engineering, etc.) are determined on a To this first calculation.
- To determine the equipment costs (Ce) the following equation was used:

$$Ce = a + bS^n$$

Where:

S: Size of the parameter used to determine the cost of the equipment

A, b and n: Constants obtained from Table 6.6 of the book "Chemical Engineering Design

- Gavin Towler"
  - The costs obtained in this way are based on equipment of the Gulf Coast (US) of the year 2006, for this reason the Chemical Engineering (IC) Cost Indices were used to obtain the cost of the equipment in the present year (2015).

$$Ce_{2015} = Ce_{2006} \, x \, \frac{IC_{2015}}{IC_{2006}}$$

Cost Index				
Year	IC			
2006	499.6			
2015	573.1			

Finally, a correction factor for location (FL) is applied to obtain the costs in Peru and a correction factor for material (FM), since the calculated equipment costs are based on carbon steel (FM = 1) and it is Necessary to determine the costs of the equipment in stainless steel 304 (FM = 1.3).

**Table 6.5.** Materials Cost Factors,  $f_{mr}$ , Relative to Plain Carbon Steel

Material	f <sub>m</sub>
Carbon steel	1.0
Aluminum and bronze	1.07
Cast steel	1.1
304 stainless steel	1.3
316 stainless steel	1.3
321 stainless steel	1.5
Hastelloy C	1.55
Monel	1.65
Nickel and Inconel	1.7

**Table 6.7.** Location Factors

Country	Region	<b>Location Factor</b>
United States	Gulf Coast	1.00
	East Coast	1.04
	West Coast	1.07
	Midwest	1.02
Canada	Ontario	1.00
	Fort McMurray	1.60
Mexico		1.03
Brazil		1.14
China	imported	1.12
	indigenous	0.61
Japan	-	1.26
SE Asia		1.12
Australia		1.21
India		1.02
Middle East		1.07
France		1.13
Germany		1.11
Italy		1.14
Netherlands		1.19
Russia		1.53
United Kingdom		1.02

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	COSTO DE EQUIPOS (Ce) ESCALADO Y LOCALIZADO CON CORRECCION DE MATERIAL (\$ del año 2015)											
					Ce	e = a + bS'	'n			IC	FL	FM = 1.3 (ss 304)
Codigo	N	Nombre del Equipo		Tamaño del Equipo (S)	Unidad es	a	b	n	Ce (\$ del año 2006 - U.S. Gulf Coast)	Ce escalado (\$ del año 2015 - U.S. Gulf Coast)	Ce escalado y localizado (\$ del año 2015 - Peru)	Ce escalado y localizado con correcion de material (\$ del año 2015 - Peru)
	Tanque de	e techo conico (almac IPA)	5	393	m3	5700	700	0.7	257,539	295,428	326,430	424,358
M-110	Mezclador de	Tanque de mezclado	1	1.9	m3	5700	700	0.7	6,810	13,585	15,011	19,514
WI-110	IPA	Mezclador de helice	1	0.30	kW	4300	1920	0.8	5,033	13,383	13,011	19,314
L-111	Bomba alimentac	Bomba centrifuga	2	1.35	L/s	3300	48	1.2	6,738	10,571	11,680	15,184
L-111	IPA	Motor a prueba de explosion	2	0.41	kW	920	600	0.7	2,477	10,571	11,080	13,164
V-112	7	Vaporizador de IPA	1	48	m2	11000	115	1	16,572	19,010	21,005	27,306
E-113	Pı	re-calentador de IPA	1	9	m2	11000	115	1	12,073	13,849	15,302	19,893
R-120		Reactor tubular	1	238	m2	11000	115	1	38,411	44,062	48,686	63,292
Q-122		Horno Cilindrico	1	1.39	MW	53000	69000	0.8	142,701	163,695	180,873	235,135
E-130		Enfriador	1	15	m2	11000	115	1	12,691	14,557	16,085	20,911
H-132		Separador de fases	1	459	kg	-10000	600	0.6	10,559	12,112	13,384	17,399
D-140	Destilador	Recipiente a presion	1	3775	kg	-10000	600	0.6	56,926	84,429	93.289	121,276
D-140	Acetona	Platos perforados	58	1.25	m	100	120	2	16,675	84,429	93,289	121,276
L-143	Bomba reflujo	Bomba centrifuga	2	2.50	L/s	3300	48	1.2	6,888	10,181	11 250	14.624
L-143	Acetona	Motor a prueba de explosion	2	0.05	kW	920	600	0.7	1,987	10,181	11,250	14,624
E-144	F	Rehervidor Acetona	1	26	m2	11000	115	1	13,958	16,011	17,691	22,999
D-150	Destilador IPA	Recipiente a presion	1	520	kg	-10000	600	0.6	11,978	18,810	20,784	27,020
D-130	Destilador IPA	Platos perforados	34	0.50	m	100	120	2	4,420	18,810	20,784	27,020
E-151	Condensador IPA		1	37	m2	11000	115	1	15,198	17,433	19,263	25,042
L-153	Bomba reflujo	Bomba centrifuga	2	0.04	L/s	3300	48	1.2	6,602	9,693	10,711	13,924
L-133	IPA	Motor a prueba de explosion	2	0.001	kW	920	600	0.7	1,848	9,093	10,711	13,924
E-154		Rehervidor IPA	1	26	m2	11000	115	1	13,956	16,009	17,689	22,995
	Tanque de t	echo conico (almac Acetona)	4	393	m3	5700	700	0.7	206,031	236,342	261,144	339,487
				Costo T	otal de E	quipos						1,430,358

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- From the costs of major equipment (Ce) we proceed to determine the other components of the Investment in Fixed Capital, for this we use a percentage within the range recommended in Table 4 of Chapter 6 of the book "Plant Design and Economics For Chemical Engineers - Max S. Peters"

COST OF FIXED CAPITAL (\$ 2015)								
Item	Range (%)	Value (%)	Cost					
<b>Direct Costs (Fixed Assets)</b>								
Equipment Cost	15 - 40	23	1,430,358					
Installation	6 - 14	10	621,895					
Control and Instrumentation	2 - 8	3	186,568					
Pipes and fittings	3 - 20	8	497,516					
Electrical equipment and supplies	2 - 10	3	186,568					
Buildings and structures	3 - 18	6	373,137					
Delimitations	2 - 5	3	186,568					
Services and Facilities	8 - 20	13	808,463					
Ground	1 - 2	1	62,189					
<b>Total Direct Costs</b>		70	4,353,263					
Indirect Costs (Intangibles)								
Engineering and supervision	4 - 21	8	497,516					
Construction expenses	4 - 16	9	559,705					
Utility of the contractor	2 - 6	4	248,758					
Contingencies	5 – 15	9	559,705					
<b>Total Indirect Costs</b>	30	1,865,684						
Total Fixed Capital		100	6,218,947					

- We are assuming that the land will be purchased at the beginning of the project, for this reason the investment of this component is recovered at the end of the project as a salvage value (Vs), since the land does not depreciate.

# 6. <u>DETERMINATION OF THE BALANCE PRICE</u>

Of the components of the total cost of the product, some of them could be determined using production data, material balance, raw material price, investment, labor, etc. From Table 27 of Chapter 6 of the book "Plant Design and Economics for Chemical Engineers - Max S. Peters" you get:

	TOTAL PRODUCT COST (C)					
	Components	Range (%)				
	Direct Costs					
	Raw Material (IPA)					
	Direct Labor (MO)					
	Supervision	(10 - 25)% MO				
	Laboratory	(10 - 20)% MO				
	Maintenance and repairs	(2 - 10)% I				
PRODUCTION OR	Services (steam, water, gas, etc.)	(10 - 20)% C				
MANUFACTURING	Patents	(0 - 6)% C				
COSTS	<b>Total Direct Costs</b>					
	Fixed Charges					
	depreciation					
	Asset tax	(1 - 4)% I				
	Insurance	(0.4 - 1)% I				
	Total Fixed Charges					
	Superintendent's Charges	(5 - 15)% C				
GENERAL	Administrative expenses	15% MO				
EXPENSES	Sales and Distribution Expenses	(2 - 20)% C				

Nominal Capacity (MTM / Year)	21.5
Service factor (%)	93.2%
TM IPA / TM Acetone	1.34

Production Program (MTM / Year)						
Production Acetone	20.0					
IPA Requirement	26.7					

- The IPA price was determined from the CIF value of the import report divided by the net import weight for the United States, accounting for 95% of the imports of this product.

Reporte de Importaciones por Subpartida Nacional/Pais Origen 2015

Subpartida Nacional: 2905.12.20.00 ALCOHOL ISOPROPILICO

País de Origen	Valor FOB(dólares)	Valor CIF(dólares)	Peso Neto(Kilos)
US - UNITED STATES	3,273,998.59	3,558,274.34	3,045,599.700
NL - NETHERLANDS	141,311.66	149,720.36	118,560.000
DE - GERMANY	33,891.59	37,242.27	4,239.360
KR - KOREA, REPUBLIC OF	29,025.04	30,539.09	25,600.000
CN - CHINA	12,566.00	14,717.09	12.811.290
MX - MEXICO	2,481.89	2,787.27	499.200
CH - SWITZERLAND	167.76	407.24	8.520
ES - SPAIN	166.50	175.36	13.980
LOS DEMAS - LOS DEMAS	0.00	0.00	0.000
TOTAL - TOTAL	3,493,609.03	3,793,863.02	3,207,332.050

For the calculation of some of the components of the cost of the product, we divide them into 3 groups: costs proportional to the level of production, costs proportional to the investment in fixed capital (I) and costs proportional to labor (MO).

PROPORTIONAL COSTS TO THE LEVEL OF PRODUCTION					
Components	Annual requirement		Unit Cost		Total cost
Raw Material (IPA)	26767	TM/year	1168	\$/TM	31,272,745

- We determine the direct labor requirement from the following graph, for which we take the line B (average conditions).

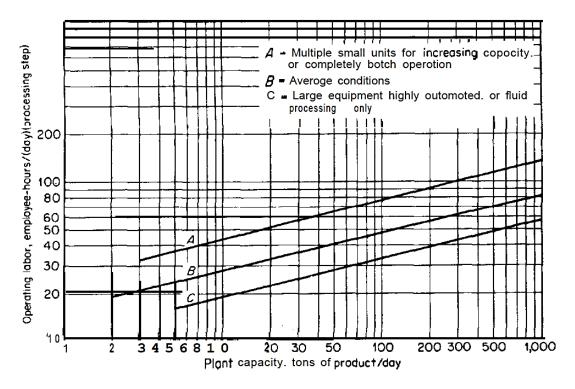


FIGURE 6-8
Operating labor requirements for chemical process industries.

DIRECT WORK HAND		
<b>H-h / DO.shift</b> 45		
Shifts	3	
DO / year	340	
H-H / year	45900	
\$ / H-H	3.0	

PROPORTIONAL COSTS TO THE LABOR				
Components	Range (%)	Value (%)	<b>Total Cost</b>	
Direct Labor (MO)	$MO = h-H/year \times h-H$		137,700	
Supervision	(10 - 25)% MO	20%	27,540	
Laboratory	(10 - 20)% MO	10%	13,770	
Administrative expenses	15% MO	15%	20,655	
Total (\$/	199,665			

- As we know the investment in fixed capital (I = Vo), we can determine the depreciation (D) assuming a 10-year project duration (N), with which the Net Funds Flow (FNF) will subsequently be determined for the entire planning horizon. As mentioned above the land is not depreciated, so it is recovered at the end of the project as a salvage value (Vs).

PROPORTIONAL COSTS TO THE LABOR				
Components	Components	Components	Components	
Direct Labor (MO)	$MO = h-H/a\tilde{n}$	$MO = h-H/a\tilde{n}o \times h-H$		
Supervision	(10 - 25)% MO	20%	27,540	
Laboratory	(10 - 20)% MO	10%	13,770	
Administrative expenses	15% MO	15%	20,655	
Total (\$	199,665			

- Finally, we determine the other components whose cost is proportional to the cost of the product (C), with which we would have an equation with a single unknown. Solving the equation we would have the following results:

	TOTAL PRODUCT COST (C)					
	Components	Range (%)	Value (%)	Total	cost	
	<b>Direct Costs</b>					
	Raw Material (IPA)			31,272,745	31,272,745	
	Direct Labor (MO)			137,700	137,700	$\mathbf{\tilde{s}}$
	Supervision	(10 - 25)% MO	20%	27,540	27,540	COSTS
	Laboratory	(10 - 20)% MO	10%	13,770	13,770	VARIABLE
	Maintenance and repairs	(2 - 10)% I	8%	497,516	497,516	ZIA
PRODUCTION OR MANUFACTURING COSTS	Services (steam, water, gas, etc.)	(10 - 20)% C	15%	0.10 C	6,384,189	VAF
	Patents	(0 - 6)% C	1%	0.01 C	425,613	
	Total Direct Costs				38,759,072	
	Fixed Charges					
	depreciation			615,676	615,676	LS
	Asset tax	(1 - 4)% I	2%	124,379	124,379	SO
	Insurance	(0.4 - 1)% I	1%	62,189	62,189	D C
	Total Fixed Charges				802,244	FIXED COSTS
	<b>Superintendent's Charges</b>	(5 - 15)% C	5%	0.05 C	2,128,063	
GENERAL	Administrative expenses	15% MO	15%	20,655	20,655	
EXPENSES	Sales and Distribution Expenses	(2 - 20)% C	2%	0.02 C	851,225	
	Total (\$	S/Año)		С	42,561,260	

To determine the price of acetone at break-even point (zero utilities), the total cost of the product would have to be equated with the sales revenue, so the price of acetone will be the total cost of the product between productions of acetone.

<b>Acetone Balance Price (ThUS \$ / TM)</b>	2.13
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# **DETERMINATION OF WORKING CAPITAL**

- We chose a period of 14 days of inventory of raw material and finished product:

Working Capital (US \$ of 2015)				
CURRENT ASSETS				
Inv. Raw Material (14 OD)				
TM / DO	78.7			
TM / Year	1102.2			
MUS\$/TM	1.17			
US\$/Year	1,287,701			
Inv. Finished Products (14 DO)				
TM / DO	58.8			
TM / Year	823.5			
MUS\$/TM	2.13			
US\$/Year	1,755,847			
Accounts Receivable (30 AD)				
MUS\$/DC	116.8			
MUS\$/Año	3,504,822			
ACT. CURRENT (US \$ / Year)	6,548,370			
CURRENT LIABILITIES				
Accounts Payable (30 AD)				
MUS\$/DC	85.7			
US\$/Year	2,570,363			
WORKING CAPITAL				
US\$/Year	3,978,007			

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# 8. ANNEXES

# ANNEX N°1

# **Mixer**

Residence time (min)	30
Mass to be stored (kg)	1268.86
Density (Kg / m3)	780
Useful volume (m3)	1.6267
Safety margin (%)	10
Design Volume (m3)	1.7894

Dimensions of the mixer	
Diameter of tank Dt (m)	1.3500
Impeller Diameter Da (m)	0.4500
Height of liquid H (m)	1.3500
Deflector thickness j (m)	0.1350
Tank free space E (m)	0.4500
Height of blade W (m)	0.0900
Shovel width L (m)	0.1125
Volume of tank V (m3)	1.9324

P heuristic (	kW)	0.19

Determination of power for Re> 10000			
P (kW)	0.30		
Fluid density (kg / m3)	780.00		
Speed of rotation n (rps)	1.25		
Impeller Diameter Da (m)	0.5067		
KT	5.80		

Viscosity (Kg / m.s)	0.0015
Reynolds number (Re)	164234.47
Velocidad de giro (m/s)	0.6333

# ANNEX N°2

# **IPA Feed Pumps**

From the following data obtained from the material balance.

Current	2	3
Temperature (° C)	33.470	33.470
Pressure (kPa)	99.80	400.00
Fraction of vapor	0	0
Molar flow (kmol / hr)	81.5159	81.5159
Components		
Molar flow (kmol / hr)		
HYDROGEN	0.0000	0.0000
ACETONE	2.1429	2.1429
IPA	52.69927795	52.69927795
H20	26.67374857	26.67374857
Mass flow (kg / h)	3772.00	3772.00
Density (kg / m3)	777.6000	777.6000
Flow rate (m3 / s)	0.00135	0.00135

Performing energy balance at pump inlet and outlet:

$$E_1 + H_B = E_2$$

$$\frac{P_1}{\gamma} + Z_1 + \frac{\overline{V}_1}{2g} + H_B = \frac{P_2}{\gamma} + Z_2 + \frac{\overline{V}_2}{2g}$$

$$H_B = \frac{P_2}{\gamma} - \frac{P_1}{\gamma} = \frac{300.2 \text{ kPa}}{9.81 \text{ N } \times 777.6 \frac{\text{kg}}{\text{m}^3}} = 39.354 \text{ m}$$

For the design, the data of the impeller diameter, roughness, and rotational speed are considered.

Design data			
Impeller Diameter Da (m)	0.371		
Pump head H (m)	39.3537		
Rotational speed n (1 / sec)	1.4		
Power of pump P (W)	404.5051971		
Discharge flow Q (m3 / s)	0.00135		
Viscosity (Kg / m.s)	0.001		
Density (Kg / m3)	777.6000		
Roughness □ (m)	0.0001		
Coefficient of capacity Cq	0.0188		
Coefficient of head Ch	1431.036		
Power factor CP	26.9721		

# ANNEX N ° 3

# Vaporizer

Energy balance:

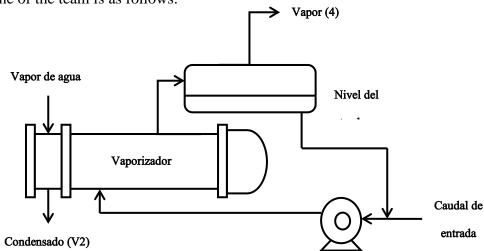
Of the following data:

# A. Heat balance.

For design considerations for a vaporizer, only 80% of the inlet flow to the schematic can be vaporized and since an outflow of 81.5159 kmol/h is required, the required flow rate of vaporizer inlet should be:

Flow rate of the vaporizer = 
$$\frac{81.5159}{0.8}$$
 = 101.8949 kmol/h

The outline of the team is as follows:



As seen in the diagram, the inlet flow to the vaporizer is a mixture of the liquid stream coming down from the drum and line 3, whereby, from an energy balance, the inlet temperature in the vaporizer is:

$$H_{Mixture \ at \ 33.47 \,^{\circ}C} \ x \ \dot{m3} + H_{Mixture \ in F.L.At \ 117.00 \,^{\circ}C} \ x \ \dot{L}$$

$$= H_{Mix \ in \ the \ feed \ to \ T} \ x \ (m3 + L)$$

From the energy balance, you get:

$$T_{feeding} = 76.08$$
 °C

For the determination of the overall transfer coefficient, we have the following calculation sequence:

# B. Determination of water vapor flow.

Required heat in the Preheating zone: From subcooled liquid to saturated liquid.

- Enthalpy of the liquid mixture at 76.08 ° C: 57372.73 kJ / kmol
- Enthalpy of the liquid mixture at 117.00 ° C: 64095.21 kJ / kmol

$$Q_p = (64095.21 - 57372.73) \times 101.8949 = 684986.43 \frac{\text{kJ}}{\text{h}}$$

Heat required in the Vaporization zone: From saturated to saturated vapor.

• Steam enthalpy of the mixture at 117.00 ° C: 100865.01 kJ / kmol

$$Q_v = (100865.01 - 64095.21) \times 81.5159 = 2997323.34 \frac{\text{kJ}}{\text{h}}$$

$$Q = Q_p + Q_v = 3682309.77 \ kJ/h$$

The required steam flow rate (165 ° C and 700 kPa):

$$\dot{m}_{water\ vapor} = \frac{3682309.77}{2072.959} = 1776.35 \ \frac{kg}{h}$$

# C. Correction of LMTD.

Since the input flow undergoes a phase change, the calculation of the LMTD will be performed in two zones:

a. Preheating zone:

$$LMTD_{p} = \frac{(438.15 K - 390.15 K) - (438.15 K - 349.23 K)}{\ln{(\frac{(438.15 K - 390.15 K)}{(438.15 K - 349.23 K)})}} = 66.37 K$$

b. Vaporization zone:

$$LMTD_{v} = 438.15 K - 390.15 K = 48.00 K$$

c. Balanced LMTD:

$$LMTD = \frac{Q_p + Q_v}{\frac{Q_p}{LMTD_p} + \frac{Q_v}{LMTD_v}} = \frac{3682309.77}{\frac{684986.43}{66.37} + \frac{2997323.34}{48.00}} = 50.61 \, K$$

# D. Determination of the global coefficient for the preheating zone.

Coefficient of heat transfer per armor - ho.

For purposes of calculation the ho recommended by Donald Kern for steam flow will be used:

$$h_o = 8000 \frac{W}{m^2 \cdot K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

Internal area of a tube: 
$$A_{tr} = \frac{\pi x Di^2}{4} = 0.00019 m^2$$

Pipe area: 
$$A_t = \frac{Nt \ x \ A_{t}}{Number \ of \ steps} = \frac{166 \ x \ 0.00019}{6} = 0.00536 \ m^2$$

Mixing Flux: 
$$G_t = \frac{2537.72 \, kg/h}{0.00536 \, m^2} = 131.50 \, \frac{kg}{s.m^2}$$

Ha  $T_{average} = \frac{76.08 + 117.70}{2} = 96.54 \,^{\circ}C$ , Properties of the fluid are:

$$\mu = 0.000361 \ Pa.s$$
  $Cp = 3.5333 \frac{kJ}{kg.K}$   $k = 0.2325 \frac{W}{m.K}$ 

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{131.50 \times 0.0157 \, m}{0.000361 \, Pa. \, s} = 5728.98$$

From Fig. 24 of Donald Kern's book "Heat Transfer Processes", Factor Jh is extracted for the given Reynolds number:

$$Jh = 18.00$$

So:

$$hi = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 469.7782 \ \frac{W}{m^2. K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{8000 \times 469.7782}{8000 + 469.7782} = 443.7218 \frac{W}{m^2 \cdot K}$$

Area required for preheating:

$$A1 = \frac{\frac{684986.43}{66.37 \times 3.6}}{443.7218} = 6.4609 \ m^2$$

# E. Determination of the overall coefficient for the vaporization zone.

• Coefficient of heat transfer per armor - ho.

For purposes of calculation the ho recommended by Donald Kern for steam flow will be used:

$$h_o = 8000 \frac{W}{m^2 \cdot K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

Internal area of a tube: 
$$A_{tr} = \frac{\pi \times Di^2}{4} = 0.00019 \text{ m}^2$$

Pipe area: 
$$A_t = \frac{Nt \ x \ A_{t'}}{Number \ of \ steps} = \frac{166 \ x \ 0.00019}{6} = 0.00536 \ m^2$$

Mixing Flux: 
$$G_t = \frac{2537.72 \, kg/h}{0.00536 \, m^2} = 131.50 \frac{kg}{s. \, m^2}$$

Ha  $T_{average} = 117.00 \,^{\circ}C$ , l the properties of the fluid are:

$$\mu = 0.000255 \, Pa. \, s$$

$$= 3.6698 \frac{kJ}{kg.K}$$

$$Cpk = 0.2253 \frac{W}{m.K}$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{131.50 \times 0.0157 \, m}{0.000255 \, Pa. \, s} = 8097.64$$

From Fig. 24 of Donald Kern's book "Heat Transfer Processes", Factor Jh is extracted for the given Reynolds number:

$$Jh = 29.00$$

So:

$$hi = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 668.7653 \ \frac{W}{m^2.K}$$

For a clean global coefficient (U2):

$$U2 = \frac{8000 \times 207.5479}{8000 + 207.5479} = 617.1724 \frac{W}{m^2.K}$$

Area required for vaporization::

$$A2 = \frac{\frac{2997323.34}{48 \times 3.6}}{617.1724} = 28.1050 \, m^2$$

# F. Checking maximum heat flow.

Total clean area Ac:

$$Ac = A1 + A2 = 6.4609 + 28.1050 = 34.5659 m^2$$

• Total balanced clean coefficient:

$$U = \frac{\frac{684986.43}{66.37 \times 3.6} + 2997323.34/(48 \times 3.6)}{34.5659} = 584.75 \frac{W}{m^2 \cdot K}$$

• Total design coefficient:

Total area = Nt x LT x RT = 
$$166 \times 6 \times 0.1963 \frac{ft^2}{ft} \times 0.3048 m$$
  
=  $59.5929 m^2$ 

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Ratio of pipe surface per linear foot (BWG 16)

From the following ratio ratio for the calculation of the design area for vaporization:

$$\frac{28.1050}{34.5659} \times 59.5929 \, m^2 = 48.4541 \, m^2$$

The heat flow in the vaporization zone is:

$$Q_F = \frac{2997323.34}{48.4541 \times 3.6} = 17183.06 \frac{W}{m2} < 78000 \frac{W}{m2}$$
 (Permissible heat flow)

If the heat flow in the vaporization zone is permissible, the conditions given for the next design are feasible.

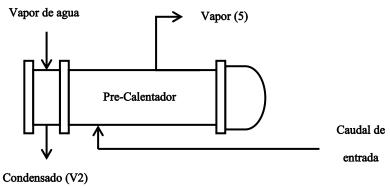
# ANNEX N°4

# **Preheater**

Energy balance: From the following data:

### G. Heat balance.

The outline of the team is as follows:



For the determination of the overall transfer coefficient, we have the following calculation sequence:

# H. Determination of the water vapor flow rate.

Required heat in the Preheating zone: From subcooled liquid to saturated liquid.

• Difference of enthalpies of the mixture in vapor phase from  $117.00 \,^{\circ}$  C to  $180.00 \,^{\circ}$  C:  $179.8906 \, \text{kJ} / \text{kg}$ 

$$Q_p = (179.8906) \times 2537.72 = 456511.97 \frac{\text{kJ}}{\text{h}}$$
 
$$Q = Q_p = 456511.97 \text{ kJ/h}$$

The required water vapor flow rate (1 ° C and 700 kPa):

$$\dot{m}_{water\ vapor} = \frac{456511.97}{1980.761} = 230.4730 \ \frac{kg}{h}$$

I. Determination of LMTD.

$$LMTD = \frac{(471.44 \, K - 453.15 \, K) - (471.44 \, K - 390.15 \, K)}{\ln \left( \frac{(471.44 \, K - 453.15 \, K)}{(471.44 \, K - 390.15 \, K)} \right)} = 42.24 \, K$$

- J. Determination of the global coefficient for the heating zone.
- Coefficient of heat transfer per armor ho.

For purposes of calculation the ho recommended by Donald Kern for steam flow will be used:

$$h_o = 8000 \frac{W}{m^2 \cdot K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

Internal area of a tube: 
$$A_{t'} = \frac{\pi \times Di^2}{4} = 0.00019 \text{ m}^2$$

Pipe area: 
$$A_t = \frac{Nt \, x \, A_{t'}}{Number \, of \, steps} = \frac{52 \, x \, 0.00019}{1} = 0.01008 \, m^2$$

Mixing Flux: 
$$G_t = \frac{2537.72 \, kg/h}{0.01008 \, m^2} = 69.96 \frac{kg}{s. \, m^2}$$

Ha  $T_{average} = \frac{180.00 + 117.00}{2} = 148.50 \,^{\circ}C$ , Properties of the fluid are:

$$\mu = 0.000010 \ Pa.s$$

$$Cp = 1.9710 \frac{kJ}{kg.K}$$

$$k = 0.0252 \frac{W}{m.K}$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{69.96 \times 0.0157 \, m}{0.000010 \, Pa. \, s} = 109812.20$$

From Fig. 24 of Donald Kern's book "Heat Transfer Processes", Factor Jh is extracted for the given Reynolds number:

$$Jh = 400.00$$

So:

$$hi = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 369.4963 \ \frac{W}{m^2. K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{8000 \times 369.4963}{8000 + 369.4963} = 353.1838 \frac{W}{m^2.K}$$

Area required for heating:

$$A1 = \frac{\frac{456511.97}{42.24 \times 3.6}}{353.1838} = 8.5011 \ m^2$$

• Total design coefficient:

Total area = Nt x LT x RT = 
$$166 \times 6 \times 0.1963 \frac{ft^2}{ft} \times 0.3048 m$$
  
=  $9.3338 m^2$ 

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Ratio of pipe surface per linear foot (BWG 16)

So:

$$UD = \frac{\frac{456511.97}{42.24 \times 3.6}}{9.3338} = 321.64 \frac{W}{m^2.K}$$

# ANNEX N°5

# Reactor

There is a tubular rectifier (PFR), in which the feed flow (F0) consists of IPA, water and acetone, and the outlet current (F), has IPA, water, DMK and H2. The characteristics of these currents are shown in the following table:

Curretnt	5	6	
Temperature (° C)	180	388	
Pressure (kPa)	360	340	
Fraction of vapor	1	1	
Molar flow (kmol / hr)	81.52	128.95	
Components			
Molar flow (kmol / hr)			
H20	26.67	26.67	
IPA	52.70	5.27	
HYDROGEN	0.00	47.43	
ACETONE	2.14	49.57	

Applying the matter balance on a differential element of the axial position (dx) in the reactor for a tube, obtaining the following differential equation:

$$F_{A0} \frac{dx_A}{(-r_A)} = dx * \frac{(1-e) * \pi * \text{Di}^2}{4}$$

$$\frac{dx_A}{dx} = \frac{(-r_A) * (1-e) * \pi * \text{Di}^2}{4 * F_{A0}} \qquad (A = IPA)$$

For the reaction:

$$IPA \rightarrow Acetone + H_2$$
  
 $H_f^{\circ} = 62900 \, kJ/kmol$ 

H<sub>f</sub>\*: Standard reaction heat.

The reaction rates are given by:

$$r_F = 22 * 10^6 . C_{IPA} . e^{-72380/RT}$$
 
$$r_R = 1000 . C_{DMK} . C_{H_2} . e^{-9480/RT}$$
 
$$r = \frac{kmol}{s.m^3 \ cat} \quad ; \quad C = \frac{kmol}{m^3 \ gas} \quad ; \quad T = K$$

The rate of reaction is determined by:

$$(-r_A) = r = r_D - r_I = 22 * 10^6$$
.  $C_{IPA}$ .  $e^{-72380/RT} - 1000$ .  $C_{DMK}$ .  $C_{H_2}$ .  $e^{-9480/RT}$ 

Applying the energy balance for a catalytic tubular reactor tube with heat exchange at steady state for a differential in the axial position (dx)

$$d(T)/d(x) = (\pi^*De^*U^*(T_{oil}-T) + \Delta Hr^*r_a^*(1-e)^*\pi^*Di^2/4)/(Fao/N^*(\Sigma\theta i^*Cpi + Xa^*\Delta Cp.))$$

Where:

Fao: IPA molar flow entering the reactor.

N: number of tubes.

Di: Internal diameter.

From: External diameter.

U: Global heat transfer coefficient

Toil: Heater oil temperature.

T: Temperature inside the tubes.

E: Empty space inside the tubes.

Θi: Mole ratio of each component in the feed relative to the reactant (IPA).

 $\Delta$ Hr: reaction enthalpy as a function of reaction temperature.

Cpi: Heat capacity of component i.

Xa: Mole fraction of the feed

# X: Axial position

On the side of the heating oil, we have a temperature profile, which is found by applying a differential energy balance with respect to the axial position (dx), we obtain the following equation:

$$d(T_{oil})/d(x) = U*\pi*De*(T-T_{oil})/(m_{oil}*Cp_{oil})$$

moil: Thermal oil mass flow.

Cpoil: Heat capacity of the thermal oil.

The thermal oil was selected Therminol VP-1, which supports a maximum temperature of  $400 \,^{\circ}$  C.

The characteristics of the oil as well as its properties are attached on the delivered CD.

The reaction enthalpy ( $\Delta$ Hr) is expressed by the following equation as a function of the reactor temperature along the tube:

$$\Delta Hr = \Delta Hr^{\circ} + \Delta H_{1} + \lambda_{vap.} + \Delta H_{v}$$

$$\Delta H_{1} = f(Cpl_{i}) \qquad \Delta Hv = f(Cpv_{i}) \qquad \Delta Hr = f(Tr_{i})$$

The expressions for heat capacities are taken as a function of temperature for each component of the Perry's Chemical Engineers' Handbook [3].

For each component in liquid phase, the equation of the heat capacity is given by:

For each component (IPA, acetone) the constants of this equation are as follows:

	IPA	C3	36.662
C1	723550	C4	-0.066395
C2	-8095	C5	0.000044064

A	cetona	C3	0.2837
C1	135600	C4	0.000689
C2	-177	C5	0

For each component (acetone, hydrogen, IPA and water) in vapor phase and / or gas:

$$\begin{split} \text{CpAce} = & 5.704*10^4 + 1.6320*10^5 * ((1.61*10^3/\text{T})/\text{Senh}(1.61*10^3/\text{T}))^2 + 9.680*10^4 * ((731.5/\text{T})/\text{Senh}(731.5/\text{T}))^2 \\ \text{CpH}_2 = & 2.762*10^4 + 9.56*10^3 * ((2.466*10^3/\text{T})/\text{Senh}(2.466*10^3/\text{T}))^2 + 3.76*10^3 * ((567.6/\text{T})/\text{Senh}(567.6/\text{T}))^2 \\ \text{CpIpa} = & 5.723*10^4 + 1.91*10^5 * ((1.4210*10^3/\text{T})/\text{Senh}(1.4210*10^3/\text{T}))^2 + 1.2155*10^5 * ((626/\text{T})/\text{Senh}(626/\text{T}))^2 \\ \text{CpW} = & 3.336*10^4 + 2.679*10^4 * ((2.6105*10^3/\text{T})/\text{Senh}(2.6105*10^3/\text{T}))^2 + 8.9*10^3 * ((1169/\text{T})/\text{Senh}(1169/\text{T}))^2 \\ \end{split}$$

The enthalpy of evaporation for each component (IPA and acetone) is given by the following equation:

 $\lambda vap. = C1*(Tr)^{(C2+C3*Tr+C4*Tr^2)}$ 

**IPA** 

C1	63080000	C3	0
C2	0.3921	C4	0

# **ACETONE**

C1	42150000	C3	0
C2	0.3397	C4	0

Where:

Tri: reduced temperature of component i, (Tebulli / Tcriticoi)

Tebulli: Boiling temperature of component i.

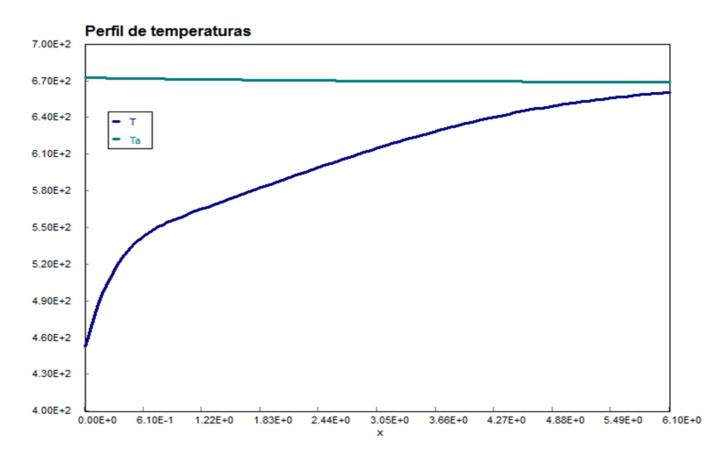
Tcriticoi: Critical temperature of component i.

For each component, the following data is available:

Component	Molar flow (kmol / hr)	Xi	θ
HYDROGEN	0	0.0000	0
ACETONE	0.03	0.0263	0.0407
IPA	53.17	0.6465	1
H20	24.368	0.3272	0.506

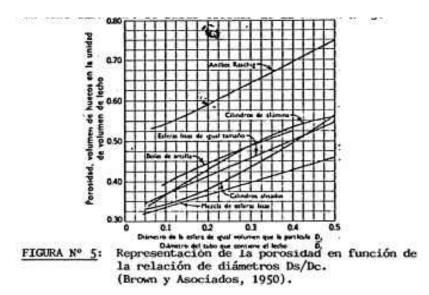
In order to solve the differential equations we used the Polymath program 6.10 (the calculations and results obtained are appended in the CD), which is described in the literature [7], for a heat transfer coefficient equal to 80 Wm-2K -1, the input temperature was taken to be  $180\,^{\circ}$  C, which is the temperature at which it leaves the preheater and the reactor output is calculated to have a temperature of 660.65 K with a conversion per step of 0.90.

The temperature profiles inside the reactor and the heating oil are obtained with the program and are plotted obtaining:



The conversion as a function of the axial position has the following graph:





The catalyst occupies a certain volume inside the reactor tubes which can be found by means of the attached graph, obtaining an empty space equal to 0.36 for compact cylinders.

The use of a fixed bed reactor with the catalyst is proposed in 0.0254 m (1 in) outer diameter tubes. It is estimated that the length of the tubes will be 6,096 m, resulting in a number of tubes equal to 490.

With the total of tubes, the volume of these in addition to the empty space can be found the mass of catalyst to be used.

$$M_{cat} = N * V_{tubo} * (1 - e) * \rho_{real} = 0.519 \ m^3 * 2000 \frac{kg}{m^3} = 1038.08 \ kg$$

The total heat exchange area is determined by the number of tubes and the external area of the tube.

$$A_{total} = N * A_{tube} = 490 * \pi * De * L = 238.36 m2$$

The power needed to reach this conversion is given by:

$$Q_{req.} = U * \overline{Cp} * (Ta_o - Ta_f) = 0.08 * 2.62798 * (400 - 396.6) = 1.244 \text{ MW}$$

### ANNEX N°6

# Thermal oil furnace

The heat requirement for the thermal oil found in the reactor design is of the order of 1,244 MW but in the furnace there are heat losses in the walls of the furnace, an acceptable value is 2% and also there are losses by gases produced by The combustion (H2O, CO2, N2 and O2 in excess) which gain heat reducing the heat yielded by the combustion, there are correlations between the efficiency of the furnace and the temperature of the output in the chimney, thus we have:

$$T_{stack} = \left\{ (0.98 - Eff) \middle/ 9.25x10^{-5} \left( 1 + \frac{ex_{air}}{100} \right)^{0.748} \right\}^{1/28}$$

$$Eff = 0.98 - 9.25x10^{-5} T_{stack}^{1128} \left( 1 + \frac{ex_{air}}{100} \right)^{0.748}$$

Where:

Tstack: temperature at the entrance of the chimney.

Eff: Oven efficiency

The outlet temperature of the gases is in the order of 25 to 40  $^{\circ}$  C higher than the inlet fluid temperature.

The incoming furnace enters a temperature of 388  $^{\circ}$  C; therefore, the temperature of the exit of the gases would be, taking a value of 420  $^{\circ}$  C (788  $^{\circ}$  F), when in addition the efficiency would be given by:

Eff: 0.896

The required heat in the oven to meet the requirement would be:

$$Q_{horno} = 1.38815 MW$$

# ANNEX N°7

# **Cooler**

From the following data:

Current	Inlet	outlet	L1	L2
Temperature (° C)	387.65	92.17	21.85	40.00
Temperature (K)	660.80	365.32	295.00	313.15
Pressure (kPa)	320.00	300.00	300.00	300.00
Fraction of vapor	1.00	1.00	0.00	0.00
Molar flow (kmol / hr)	128.9453	128.9453	2066.9000	2066.9000
Components				
Molar flow (kmol / hr)				
H20	26.6737	26.6737	2066.9000	2066.9000
IPA	5.2699	5.2699	0.0000	0.0000
HYDROGEN	47.4294	47.4294	0.0000	0.0000
ACETONE	49.5722	49.5722	0.0000	0.0000
Molar fractions				
H20	0.2069	0.2069	1.000	1.000
IPA	0.0409	0.0409	0.000	0.000
HYDROGEN	0.3678	0.3678	0.000	0.000
ACETONE	0.3844	0.3844	0.000	0.000
Mass flow (kg / h)	3772.00	3772.0042	37235.4823	37235.4823

# K. Determination of the water vapor flow rate.

The required heat for inlet flow condensation is:

$$Q_p = 2490000 \frac{\text{kJ}}{\text{h}}$$

The required cooling water flow rate (165 °C y 700 kPa):

$$\dot{m}_{water\,vapor} = \frac{2490000}{66.8717} = 37235.48227 \frac{kg}{h}$$

#### L. Determination of LMTD.

$$LMTD = \frac{(298.15 \, K - 295.00 \, K) - (313.15 \, K - 660.80 \, K)}{\ln \left( \frac{(298.15 \, K - 205.00 \, K)}{(313.15 \, K - 660.80 \, K)} \right)} = 173.53 \, K$$

#### M. Determination of the overall coefficient.

Coefficient of heat transfer per armor - ho.

Outer tube diameter: 
$$D_o = 0.0191 \, m^2$$

Separation between Pitch and Do: 
$$C' = 0.0064 \text{ m}^2$$

Armor Diameter: 
$$D_c = 0.3048 m (12 pulg.)$$

Space between baffles: 
$$B = 0.0610 m$$

Armored area: 
$$As = \frac{0.0064 \times 0.3048 \times 0.0610}{0.0254} = 0.0047 \text{ m}^2$$

Water mass flow: 
$$G_t = \frac{37235.48 \frac{kg}{h.m2}}{0.0047 m^2 x 3600} = 2209.268 \frac{kg}{s.m^2}$$

 $Taverage = 30.93 \,^{\circ}C$ , the properties of the cooling water are:

$$\mu = 0.00076 \, Pa.s$$

$$Cp = 4.2267 \frac{kJ}{kg.K}$$

$$k = 0.6217 \; \frac{W}{m.\,K}$$

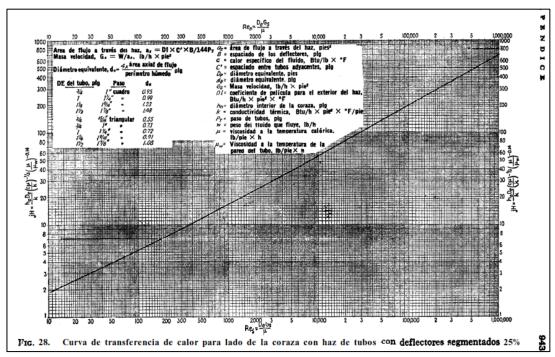
The equivalent diameter of the armor:

$$De = 4x \left( \frac{0.8661 \, x \left( \left( \left( \frac{0.0254}{0.0254} \right) \right)^2 - \frac{\pi}{4} \, x \left( \frac{0.0191}{0.0254} \right)^2 \right)}{\pi \, x \left( \frac{0.0191}{0.0254} \right)} \right) x \, 0.0254 \, = 0.01815 \, m$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{2209.268 \times 0.01815 \, m}{0.00076 \, Pa. \, s} = 53441.54$$

From Fig. 28 of Donald Kern's book "Heat Transfer Processes", the Factor Jh is extracted for the given Reynolds number:



Jh = 135.00

So:

$$Ho = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 22901.2898 \frac{W}{m^2. K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

Internal area of a tube: 
$$A_{t'} = \frac{\pi x Di^2}{4} = 0.00019 m^2$$

Pipe area: 
$$A_t = \frac{Nt \ x \ A_{t'}}{Number \ of \ steps} = \frac{82 \ x \ 0.00019}{1} = 0.01589 \ m^2$$

Mixing Flux: 
$$G_t = \frac{3772 \, kg/h}{0.01589 \, m^2} = 65.95 \, \frac{kg}{s. \, m^2}$$

 $T_{average} = \frac{387.65 + 92.17}{2} = 239.91 \,^{\circ}C$ , Properties of the fluid are:

$$\mu = 0.000017 \ Pa.s$$

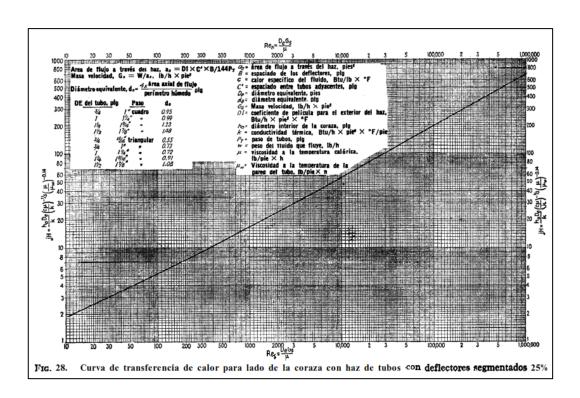
$$Cp = 4.0566 \frac{kJ}{kg.K}$$

$$k = 0.0370 \frac{W}{m.K}$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{65.95 \times 0.0157 \, m}{0.000017 \, Pa. \, s} = 60705.38$$

From Fig. 24 of Donald Kern's book "Heat Transfer Processes", Factor Jh is extracted for the given Reynolds number:



$$Jh = 160.00$$

So:

$$hi = Jh \ x \ \frac{k}{De} \ x \ \left(\frac{C \ \mu}{k}\right)^{1/3} = 464.7955 \ \frac{W}{m^2. K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{22901.2898 \times 464.7955}{22901.2898 + 464.7955} = 455.5498 \frac{W}{m^2 \cdot K}$$

Area required for heating:

$$A1 = \frac{2490000}{\frac{170.61 \times 3.6}{455.5498}} = 8.8993 \ m^2$$

### N. Checking maximum flow of heat.

• Total clean area Ac:

$$Ac = A1 = 8.8993 m^2$$

• Total design coefficient:

Total area = Nt x LT x RT = 82 x 3 x 0.1963 
$$\frac{ft^2}{ft}$$
 x 0.3048 m = 14.7187  $m^2$ :

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Tube surface ratio per linear foot (BWG 16)

$$U = \frac{\frac{2490000}{170.61 \times 3.6}}{14.7187} = 275.4374 \frac{W}{m^2 \cdot K}$$

### ANNEX N°8

### Phase separator

In a phase equilibrium with multicomponent system, the equilibrium in the vapor phase and the liquid phase following the relationship:

$$y_i = K_i * x_i$$

Where Ki is a function of the drum pressure as well as the temperature and compositions.

Since it is a non-ideal mixture it is necessary to use the Ki corrected with the activity and fugacity of each component, for which a thermodynamic model is used, the model to be used for this kind of non-ideal mixture is the UNIQUAC package.

The conditions at which the separator operates are 300 kPa and 32 °C, the equilibrium constants (Ki) are using the Aspen Hysys 8.8 simulator database, using the aforementioned thermodynamic package; for the feed stream defined by pressure, temperature and composition, the following Ki values were obtained.

<b>EQUILIBRIUM DATA (Ptamb., Ttamb.)</b>		
	K	
Hydrogen	2191.73	
Acetone	0.17	
IPA	0.05	
Water	0.04	

Now for the phase equilibrium in the separation column, by means of a material balance we obtain that:

$$F * z_i = L * x_i + V * y_i$$

Replacing the relationship between the molar fractions of the vapor and liquid the balance equation will take the following form:

$$F * z_i = L * x_i + V * K_i * x_i$$

Xi is cleared and knowing that L = F-V, the expression would remain:

$$x_i = \frac{z_i}{1 + (K_i - 1) * \frac{V}{F}}$$

Where: V / F is the vaporized fraction.

For both phases you have to satisfy that the sum of your mole fractions are equal to 1 is why if we subtract both expressions we would have:

$$f\left(\frac{V}{F}\right) = \sum_{i=1}^{c} \frac{(K_i - 1) * z_i}{1 + (K_i - 1) * \frac{V}{F}} = 0$$

This expression is called; Rachford-Rice's equation to find this the vaporized fraction must be proceeded by a numerical method for its calculation.

For the following feeding conditions:

MOLAR FEED FLOW			
F (kmol/h)	128.95		
Composition	$\mathbf{Z}_{\mathbf{f}}$		
Hydrogen	0.368		
Acetone	0.384		
IPA	0.041		
Water	0.207		

Solving the above equation is the vaporized fraction and the compositions in the liquid and vapor, the vaporized fraction is obtained by the convergence of the equation presented above.

#### Balance de materia:

	V/F	0.415	
	MOLAR LIQUID	MOLAR OF STEAM	
	FLOW	FLOW	
	75.45	53.50	
	MOLAR LIQUID	MOLAR VAPOR	
	COMPOSITION	COMPOSITION	
Hydrogen	0.0004	0.8860	
Acetone	0.5871	0.0986	
IPA	0.0675	0.0033	
Water	0.3449	0.0121	

With the calculated values, proceed to the design of the vertical drum of the separator using the following empirical equations:

Maximum permissible speed - Uperm. (Feet): 
$$\mathbf{u}_{perm} = \mathbf{K}_{tamb} \sqrt{\frac{\rho_L - \rho_v}{\rho_v}}$$

This velocity is found by the relation of the densities of the phases as well as the drum type, represented by Ktamb, by means of the Blackwell correlation, according to the following values:

$$K_{tamb} = \exp[A + B \ln F_{lv} + C(\ln F_{lv})^2 + D(\ln F_{lv})^3 + E(\ln F_{lv})^4] \qquad \text{donde } F_{lv} = \frac{W_L}{W_v} \sqrt{\frac{\rho_v}{\rho_L}}$$

WHERE		
A	-1.8774781	
В	-0.81458046	
C	-0.18707441	
D	-0.01452287	
Е	-0.00101485	

Calculate the values to find the Ktamb.

Wliq	1521.8
Wvap	192.8
Fjv	0.270

Where:

Wliq: Liquid mass flow

Wvap: Steam mass flow

	feet/s	m/s
Uperm	9.705	2.958
Ktamb	0.332	0.101

The maximum permissible speed is transformed to find the transverse area:

$$V = \frac{U_{perm} * 3600 * A_c * \rho_v}{PM_V}$$

$$A_c = \frac{PM_V*V}{U_{perm}*3600*\rho_v}$$

$0.0425 \text{ m}^2$

The diameter for the vertical drum is obtained:

Choosing a commercial diameter value of 10 "nominal diameter, 80, its internal diameter is 0.243 m.

Establish the length / diameter ratio, either by an approximate rule or with the volume necessary to contain strokes of liquid flow. For vertical flash distillation drums, the approximate rule is that hf/D is from 3.0 to 5.0. The appropriate value of hf/D within this range can be relative to the pressure in the separation tank, for design pressure the L / D should take the value of 5.

The drum height above the feed nozzle shaft, hv, should be 36 in. Plus half the diameter of the feed tube.

The depth of liquid hL can be determined from the desired reserve volume, V.

$$h_L = \frac{4 * Fvap * tr}{\pi * Di^2}$$

Dónde:

Fvap: Volumetric flow of the liquid (m<sup>3</sup>/h)

Tr: Residence time

With an hf / D ratio of 5 and a residence time of 2 minutes, the following results are obtained:

DRUM HEIGHT			
D feed (m)	0.02540		
HV (m)	0.826		
Hf (m)	1.214		
HL (m)	3.008		
Htotal (m)	5.048		

With the dimensions of the phase separating tank of 0.243 m diameter by 5.048 m in height, and for the nominal diameter 10 " 80 schedule, the thickness of the tower is 1.51 cm, in addition to the density of stainless steel 304 which is 7.9 g / cm 3, the weight of the separator with which the equipment is supplied is obtained by equation:

$$m_{armor} = \pi * Di * H_{total} * e * \rho_{steel}$$
 
$$m_{armor} = 459.08 \text{ Kg}$$

# ANNEX N°9

## **Distillation Tower of Acetone**

- Knowing the composition of the feed stream (F), we define acetone as light key (LK) and isopropyl alcohol (IPA) as heavy key (HK), whose compositions depend on the separation to be made.

Molar composition and molar fluxes of DISTILLATE and FUNDS					
Components	F (kmol/h)	D (kmol/h)	B (kmol/h)	хD	хB
Hydrogen	0.0305	0.0305	0.0000	0.0007	0.0000
Acetone	44.2993	42.1564	2.1429	0.9983	0.0645
IPA	5.0940	0.0422	5.0518	0.0010	0.1521
Water	26.0252	0.0000	26.0252	0.0000	0.7834
TOTAL	75.4490	42.2291	33.2199	1.0000	1.0000

- We determine the dew and bubble temperature of the 3 currents entering and leaving the tower, as they will be necessary in the design of the condenser and reboiler. The procedure to be performed for both the spray point and bubble is the same for any current, in this calculation will be used the values of distribution coefficients (Ki) of the Aspen Hysys simulator database for each current defined by its pressure, Temperature and composition.

- Proceeding in the same way with the other currents you get:

CURRENT	P(kPa)	T <sub>burb</sub> (°C)	Trocio (°C)
Feeding	300	38.20	103.00
Distilled	280	45.78	89.25
Money	300	107.00	125.90

- We applied the ShortCut Method to determine the number of ideal dishes (Nid) for a reflux (R = 1.25Rm), the feed plate (NF), the minimum number of plates (Nm) and minimum reflux tower. The first step is to verify if the components are distributed as initially assumed, for this the Shiras equation:

Bubble Point supply			Tempera	ture (°C)	Pressur	re (kPa)
It is iterated until:	1/∑α.xi - Kr	0.0000	38.20		300	
Components	F (kmol/h)	xi	Ki	$\alpha = Ki/Kr$	α.xi	yi
Hydrogen	0.0305	0.0004	2111	30869.84	12.4794	0.8532
Acetone	44.2993	0.5871	0.2134	3.12	1.8326	0.1253
IPA	5.0940	0.0675	0.0684	1.00	0.0675	0.0046
Water	26.0252	0.3449	0.0490	0.72	0.2471	0.0169
TOTAL	75.4490	1.0000			14.6266	1.0000

Dew Point supply			Temperature (°C)		Pressure (kPa)	
It is iterated until:	$\sum (yi/\alpha) - Kr$	0.0000	103.00		30	00
Components	F (kmol/h)	yi	Ki	$\alpha = Ki/Kr$	yi/α	xi
Hydrogen	0.0305	0.0004	11797	3718.58	0.0000	0.0000
Acetone	44.2993	0.5871	5.3974	1.70	0.3451	0.1088
IPA	5.0940	0.0675	3.1725	1.00	0.0675	0.0213
Water	26.0252	0.3449	0.3965	0.12	2.7599	0.8699
TOTAL	75.4490	1.0000			3.1725	1.0000

$$\frac{x_{JD}D}{z_{JF}F} = \left(\frac{\alpha_J - 1}{\alpha_{lk} - 1}\right) \frac{x_{lkD}D}{z_{lkF}F} + \left(\frac{\alpha_{lk} - \alpha_J}{\alpha_{lk} - 1}\right) \frac{x_{hkD}D}{z_{hkF}F}$$

- A component will be distributed if  $0 \le xJDD / zJFF \le 1$ , therefore:
- We calculate the minimum backflow (Rm) using the Underwood method, for this it is necessary to determine the thermal condition of the feed mixture ("q") and the value of  $\varphi$  obtained by iterating for values between the  $\alpha$  Components.

Enthalpy of the feeding			
Temperature (°C)	32		
H <sub>F</sub> (kJ/kmol)	-2.641E+05		
H <sub>G</sub> (kJ/kmol)	-2.242E+05		
H <sub>L</sub> (kJ/kmol)	-2.648E+05		

$$q = \frac{H_G - H_F}{H_G - H_L}$$

$$q = \frac{H_G - H_F}{H_G - H_L}$$

$$q = \frac{-2.242 - (-2.641)}{-2.242 - (-2.648)} = 1.0173$$

Key component check					Tav	(°C)
We assume $Ki = [(Ki)_{top.}(Ki)_{bot}]^{0.5}$					77.	.63
Components	F (kmol/h)	D (kmol/h)	Ki	$\alpha = Ki/Kr$	$X_{JD}.D/Z_{JF}.F$	Distribute?
Hydrogen	0.0305	0.0305	2710	1964.04	3657.60	No
Acetone	44.2993	42.1564	2.08	1.51	0.9516	Si
IPA	5.0940	0.0422	1.38	1.00	0.0083	Si
Water	26.0252	0.0000	0.72	0.52	-0.8786	No
TOTAL	75.4490	42.2291				

The values of q and  $\varphi$  are replaced in the following equations:

$$\sum \frac{\alpha_J z_{JF} F}{\alpha_J - \phi} = F(1 - q) \qquad \qquad \sum \frac{\alpha_J x_{JD} D}{\alpha_J - \phi} = D(R_m + 1)$$

Calculation of the	φ=	1.0428		
For supply q =	1.0173	1 - q -	$1 - q - \sum \alpha . z F/(\alpha - \varphi) =$	
Components	Ki	$\alpha = Ki/Kr$	$\alpha.zF/(\alpha-\phi)$	$[\alpha.xD/(\alpha-\phi)].D$
Hydrogen	2710	1964.04	0.0004	0.0305
Acetone	2.08	1.51	1.9081	137.0033
IPA	1.38	1.00	-1.5774	-0.9859
Water	0.72	0.52	-0.3484	0.0000
TOTAL			-0.0173	136.0479

D(Rm+1)	136.0479
Rm	2.2217

The minimum number of plates (Nm) is determined by the equation of Fenske:

$$N_{m} = \frac{\log \left[ \left( \frac{x_{lk}}{x_{hk}} \right)_{D} \left( \frac{x_{hk}}{x_{lk}} \right)_{B} \right]}{\log(\alpha_{lkAV})} - 1$$

αlkAV	1.51
Nm	17.95

$$\alpha_{lkAV} = \sqrt{\left(\frac{K_{lk}}{K_{hk}}\right)_D \left(\frac{K_{lk}}{K_{hk}}\right)_B}$$

- The number of ideal dishes (Nid) for a given reflux ratio (R = 1.25Rm) is determined by the correlation of Gilliland:

$$X = \frac{R - R_m}{R + 1}$$

$$\frac{N - N_{\rm m}}{N + 1} = 1 - e^{\left[\frac{1 + 54.4X}{11 + 117.2X} \left(\frac{X - 1}{X^{0.5}}\right)\right]}$$

R/Rm	1.25
R	2.78
X = (R - Rm)/(R + 1)	0.15
(N-Nm)/(N+1)	0.51
Nid	37.51

- The Kirkbride equation gives an approximate location of the feed plate:

$$\frac{N_R}{N_S} = \left[ \left( \frac{z_{hkF}}{z_{lkF}} \right) \left( \frac{x_{lkB}}{x_{hkD}} \right) \left( \frac{B}{D} \right) \right]^{0.206}$$

NR/NS	3.39
NR	28.97
NS	8.54

- For the design of perforated plates of cross-flow of a single step was taken into consideration the maximum flows of both liquid and vapor in the tower located in the area of impoverishment (bottom of the tower), in addition were used the equations of the book "Mass Transfer Operations - Robert E. Treybal, Chapter 6".

	COMPOSITION AND MOLAR FLUX OF LIQUID					
	L (kmol/s)	0.0535				
Nº	COMPONENTS	M (kg/kmol) xi Li (kmol/h				
1	Hydrogen	2.016	0.0000	0.0000		
2	Acetone	58.080	0.8378	161.3709		
3	IPA	60.090	0.0271	5.2112		
4	Water	18.016	0.1351	26.0252		
Ma	average (kg/kmol)	52.72	52.72	192.6073		

COMPOSITION AND MOLAR FLOW OF STEAM		
G (kmol/s)	0.0443	

Nº	COMPONENTS	M (kg/kmol)	yi	Gi (kmol/h)
1	Hydrogen	2.016	0.0000	0.0000
2	Acetone	58.080	0.9990	159.2280
3	IPA	60.090	0.0010	0.1594
4	Water	18.016	0.0000	0.0000
Ma	verage (kg/kmol)	58.08	58.08	159.3874

- The physical properties of the fluids were obtained from the Aspen Hysys simulator database for each stream defined by its composition at the bottom of the tower and at the bubble and dew point temperature.

CONDITIONS OF OPERATION					
P (kPa) Pressure 300					
g (m/s2)	Gravity	9.807			

PHYSICAL PROPERTIES OF FLUIDS				
ρG (kg/m3)	Vapor Density	5.742		
ρL (kg/m3)	Liquid Density	710.7		
μG (kg/m.s)	Viscosity of steam	8.06E-06		
σ (N/m)	Surface tension	0.022		
μL (kg/m.s)	Viscosity liq alimentac	2.10E-04		

- The following initial characteristics of the dish were taken from which the dimensions of the tower are calculated, as well as checking that there are no operational problems (flooding, whining, dragging, etc.).

PLATE CHARACTERISTICS			OBSERVATIONS
do (m)	Diameter of the hole	0.0045	Tabla 6.2 - Item 2
p' (m)	Distance between holes	0.0135	p' = (2.5 - 5).do
t (m)	Spacing Tower	0.30	Tabla 6.1 - Item 1

- The following preliminary flow calculations were performed:

$$\begin{split} G' &= G.\,\overline{M}_{avgG} = 2.572\,kg/s & Q = \frac{G'}{\rho_G} = 0.45\,m^3/s \\ \\ L' &= L.\,\overline{M}_{avgL} = 2.821\,kg/s & q = \frac{L'}{\rho_I} = 3.97\,x\,10^{-3}\,m^3/s \end{split}$$

## **Diameter of Tower (T):**

- An orifice diameter of = 4.5 mm has been taken on an equilateral triangle distribution with distances of p = 13.5 mm between the centers of the holes.

$$\frac{A_o}{A_a} = 0.907 \left(\frac{d_o}{p'}\right)^2 = 0.1008 \ge 0.1$$
 (Equation 6.31)

- From Table 6.2 - Item 1 we determine the ranges for the calculation of the constants  $\alpha$  and  $\beta$ , considering a spacing of t = 0.30 m.

$$\frac{L'}{G'} \Big( \frac{\rho_G}{\rho_L} \Big)^{0.5} = 0.0986 \ \in [0.01 - 0.1] \qquad \text{(Use values in 0.1)}$$

$$\alpha = 0.0744 t + 0.01173 = 0.0341$$

$$\beta = 0.0304 t + 0.015 = 0.0241$$

- For the calculation of the flooding constant (CF), values of (L / G ') ( $\rho$ G /  $\rho$ L) 0.5 equal to 0.1, since it is in the range of 0.01 to 0.1.

$$C_{\rm F} = \left[\alpha \log \frac{1}{(L'/G')(\rho_{\rm G}/\rho_{\rm L})^{0.5}} + \beta\right] \left(\frac{\sigma}{0.020}\right)^{0.2} = 0.0592$$
 (Equation 6.30)

$$V_F = C_F \left(\frac{\rho_L - \rho_G}{\rho_G}\right)^{1/2} = 0.66 \text{ m/s}$$
 (Equation 6.29)

- Using 80% of the flood velocity  $V = 0.80 \quad [V] \quad F = 0.52 \text{ m/s}$ 

$$A_n = \frac{Q}{V} = 0.853 \text{ m}^2$$

- We choose a length of the spill W=0.80~T, therefore from Table 6.1 - Item 4  $A_d=0.14145~At$ 

$$A_n = A_t - A_d = A_t - 0.14145 At = (1 - 0.14145) A_t$$

$$A_t = \frac{A_n}{1 - 0.14145} = 0.994 \text{ m}^2$$

$$T = \sqrt{\frac{4A_t}{\pi}} = 1.125 \text{ m}$$

- We choose T ^ '= 1.25 m as the diameter of the tower and proceed to correct the total area previously calculated:

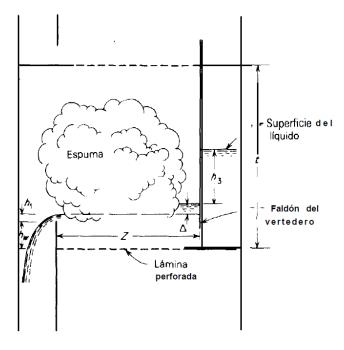
$$A'_t = \frac{\pi T'^2}{4} = 1.227 \text{ m}^2$$

$$W = 0.80 \text{ T}' = 1.00 \text{ m}$$

$$A_d = 0.14145 \, A_t{}' = 0.1736 \, m^2$$

- From Table 6.2 - Item 4 for a T  $^{\prime}$  = 1.25 m is obtained  $A_a = 0.70 A_t' = 0.8590 \text{ m}^2$ , therefore checking the flow of the liquid:

$$\frac{q}{W} = 0.004 \frac{m^3}{m.s} < 0.015 \frac{m^3}{m.s}$$
 (0. K.)



# **Depth of Liquid** $(hw + h_1)$ :

- We assume a height of the overflow (hW) of:

$$h_W = 50 \text{ mm}$$

- Iterate until  $h_1 = h_1'$ , for  $h_1 = 17.0$  mm in Equation 6.34:

$$\left(\frac{W_{eff}}{W}\right)^2 = \left(\frac{T}{W}\right)^2 - \left\{ \left[\left(\frac{T}{W}\right)^2 - 1\right]^{0.5} + \frac{2h_1}{T}\frac{T}{W}\right\}^2$$

$$W_{\rm eff} = 0.9736 \, \text{m}$$

- Replacing in Equation 6.33:

$$h_1' = 0.666 \left(\frac{q}{W}\right)^{2/3} \left(\frac{W}{W_{eff}}\right)^{2/3}$$

$$h_1' = 17.0 \text{ mm}$$

- Check the depth of the liquid:

$$h_W + h_1 = 67.0 \text{ mm} = 0.0670 \text{ m}$$

$$50 \text{ mm} < h_W + h_1 < 100 \text{ mm}$$
 (0. K.)

#### **Pressure Drop for Gas (hg):**

- From Table 6.2 - Item 2 for a do = 4.5 mm and a stainless steel tower yields 1 / do = 0.43, therefore the orifice coefficient (Co) will be:

$$C_o = 1.09 \left(\frac{d_o}{l}\right)^{0.25} = 1.346$$
 (Equation 6.37)

- From Equation  $6.31A_o/A_a = 0.1008$ , therefore  $A_o = 0.0866 \text{ m}^2$  and the gas velocity through the holes will beV<sub>o</sub> = Q/A<sub>o</sub> = 5.2 m/s.
- We calculate the Reynolds number (Re) and the Fanning friction factor (f), knowing that the absolute roughness for stainless steel is  $\varepsilon = 0.002$  mm.

$$Re = \frac{d_o. V_o. \rho_G}{\mu_G} = 16586$$

$$f = \frac{1}{4} \left\{ -1.8 \log \left[ \frac{6.9}{Re} + \left( \frac{\epsilon/d_o}{3.7} \right)^{1.11} \right] \right\}^{-2} = 0.00693$$

- Calculate the pressure drop on dry plate (hD) with Equation 6.36:

$$h_{D} = \frac{C_{o}V_{o}^{2}\rho_{G}}{2g\rho_{L}} \left[ 0.40 \left( 1.25 - \frac{A_{o}}{A_{n}} \right) + \frac{4lf}{d_{o}} + \left( 1 - \frac{A_{o}}{A_{n}} \right)^{2} \right] = 0.0190 \text{ m}$$

We determine the average flow width z = (T + W)/2 = 1.125 m and the speed in base of the active area $V_a = Q/A_a = 0.521$  m/s, therefore from Equation 6.38 we calculate the pressure drop of the liquid (hL).

$$h_L = 6.10 \times 10^{-3} + 0.725 h_W - 0.238 h_W V_a \rho_G^{0.5} + 1.225 \frac{q}{z} = 0.0318 \text{ m}$$

- The residual pressure drop (hR) is calculated from Equation 6.42:

$$h_{R} = \frac{6\sigma g_{c}}{\rho_{L} d_{o} g} = 0.0042 \text{ m}$$

- Therefore the pressure drop for the gas (hG) will be:

$$h_G = h_D + h_L + h_R = 0.0550 \ m$$

$$\Delta P_G = \rho_L g h_G = 356.1 Pa$$

#### **Flood Verification**

- Considering a 40 mm seal, we determine the smaller of two areas (Ada), the cross section of the landfill (Ad) or the free area between the landfill and the plate:

$$A_d = 0.1736 \text{ m}^2$$
  $A_{free} = W(h_W - 0.04) = 0.0100 \text{ m}^2$ 

$$A_{da} = A_{free} = 0.0100 \text{ m}^2$$

- Calculate the pressure drop at the liquid inlet (h2) of Equation 6.43.

$$h_2 = \frac{3}{2g} \left(\frac{q}{A_{da}}\right)^2 = 0.0241 \text{ m}$$

- Therefore the difference in the level of the liquid inside and outside the landfill will be:

$$h_3 = h_G + h_2 = 0.0791 \text{ m}$$

- Finally verifying the flood:

$$h_W + h_1 + h_3 = 0.1461 \text{ m} < \frac{t}{2}$$
 (0. K.)

#### **Whining Checking**

- From Table 6.1 Item 4 for a  $W=0.80\,\mathrm{T}$  is obtainedZ/2 = 0.1991T, thereforeZ = 0.498 m.
- We calculate the speed (V<sub>ow</sub>) of Equation 6.46.

$$V_{oW} = \frac{0.0229 \sigma g_c}{\mu_G} \left( \frac{{\mu_G}^2}{\sigma g_c \rho_G d_o} \frac{\rho_L}{\rho_G} \right)^{0.379} \left( \frac{l}{d_o} \right)^{0.293} \left( \frac{2 A_a d_o}{\sqrt{3} p'^3} \right)^{2.8/(Z/d_o)^{0.724}} = 1.42 \text{ m/s}$$

- whining check:

$$V_o = 3.08 \,\text{m/s} > V_{oW}$$
 (0. K.)

### **Liquid Crawl Verification**

- To determine the drag (E) we will use Figure 6.17, for which we enter by the abscissa with the value of:

$$\frac{L'}{G'} \Big( \frac{\rho_G}{\rho_L} \Big)^{0.5} = 0.10$$

- Up to the curve  $V / (V_F = 0.80)$ , therefore of the figure: E = 0.03
- The drag is so small that it does not significantly modify the hydraulics of the plate.

## **Plate Global efficiency**

- To determine the overall efficiency of the plate (Eo) we will use Figure 6.25, for which we enter by the abscissa with the value of:

$$\alpha_{AV}\mu_L = 3.2 \times 10^{-4}$$

- Therefore of the figure: Eo = 0.65

TOWER DISTILLATION IPA				
T (m)	Diameter of the tower	1.25		
Nr	Number of actual dishes	58		
Nf	Food dish	14		
H (m)	Tower height	17.10		
e (mm)	Wall Thickness	7		
M (kg)	Mass of cover	3775		

# ANNEX N°10

# **Acetone reflux pumps**

From the following data obtained from the material balance.

Current	Recycling of acetone		
Temperature (° C)	45.780	45.780	
Pressure (kPa)	260.00	280.00	
Fraction of vapor	0	0	
Molar flow (kmol / hr)	117.19	117.19	
Components			
Molar flow (kmol / hr)			
HYDROGEN	0	0	
ACETONE	117.072	117.072	
IPA	0.117	0.117	
H20	0	0	
Mass flow (kg / h)	6806.56	6806.56	
Density (kg / m3)	756.6000	756.6000	
Flow rate (m3 / s)	0.00250	0.00250	

Performing energy balance at pump inlet and outlet:

$$E_1 + H_B = E_2$$

$$\frac{P_1}{\gamma} + Z_1 + \frac{\overline{V}_1}{2g} + H_B = \frac{P_2}{\gamma} + Z_2 + \frac{\overline{V}_2}{2g}$$

$$H_B = \frac{P_2}{\gamma} - \frac{P_1}{\gamma} = \frac{300.2 \text{ kPa}}{9.81 \text{ N x 777.6 } \frac{\text{kg}}{\text{m}^3}} = 39.354 \text{ m}$$

For the design, the data of the impeller diameter, roughness and rotational speed are considered.

Design data				
Impeller Diameter Da (m)	0.371			
Pump head H (m)	2.6946			
Rotational speed n (1 / sec)	1.4			
Power of pump P (W)	49.979145			
Discharge flow Q (m3 / s)	0.00250			
Viscosity (Kg / m.s)	0.001			
Density (Kg / m3)	756.6000			
Roughness □ (m)	0.0001			
Coefficient of capacity Cq	0.0350			
Coefficient of head Ch	97.985			
Power factor CP	3.4251			

# ANNEX N°11

# Acetone column bottom reboiler

From the following data:

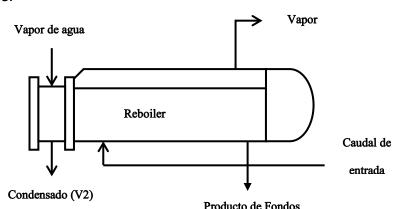
Current	V	В	V + B	V1	V2
Temperature (° C)	107.00	107.00	106.5	165.00	165.00
Temperature (K)	380.15	380.15	379.65	438.15	438.15
Pressure (kPa)	300.00	300.00	300	700.00	700.00
Fraction of vapor	1.00	0.00	0.00	1.00	0.00
Molar flow (kmol / hr)	159.5026	33.2199	192.7225	248.7051	248.7051
Components					
Molar flow (kmol / hr)					
H20	61.80	26.03	87.83	248.7051	248.7051
IPA	53.24	5.05	58.29	0.0000	0.0000
HYDROGEN	0.00	0.00	0.00	0.0000	0.0000
ACETONE	44.46	2.14	46.61	0.0000	0.0000
Molar fractions					
H20	0.3875	0.7834	0.4557	1.000	1.000
IPA	0.3338	0.1521	0.3024	0.000	0.000
HYDROGEN	0.0000	0.0000	0.0000	0.000	0.000
ACETONE	0.2788	0.0645	0.2418	0.000	0.000
Mass flow (kg / h)	6895.0937	896.8992	7791.9928	4476.6925	4476.6925

#### A. Heat balance.

For design considerations for a vaporizer, only 80% of the inlet flow to the schematic can be vaporized:

$$Vapor\ Ratio = \frac{159.5026}{192.7225} = 0.8276$$

The outline of the team is as follows:



For the determination of the overall transfer coefficient, we have the following calculation sequence:

### B. Determination of water vapor flow.

The heat required for the vaporization of the inlet flow is:

$$Q_p = 9280000 \frac{kJ}{h}$$

The required steam flow rate (165 ° C and 700 kPa):

$$\dot{m}_{water\ vapor} = \frac{9280000}{2072.959} = 4476.6925 \ \frac{kg}{h}$$

#### C. Determination of LMTD.

Since the heating medium (water vapor) has a constant temperature profile, it is feasible to calculate the LMTD as follows:

$$LMTD = \frac{(438.15 K - 380.15 K) - (438.15 K - 379.65 K)}{\ln \left( \frac{(438.15 K - 380.15 K)}{(438.15 K - 379.65 K)} \right)} = 58.2496 K$$

#### D. Determination of the overall coefficient.

• Coefficient of heat transfer per armor - ho.

Outer tube diameter: 
$$D_o = 0.0191 \, m^2$$

Separation between Pitch and Do:  $C' = 0.0064 \text{ m}^2$ 

Armor Diameter: 
$$D_c = 0.3366 \text{ m} (13.25 \text{ pulg.})$$

Space between baffles: B = 0.0673 m

Armored area: 
$$As = \frac{0.0048 \times 0.3366 \times 0.0673}{0.0254} = 0.0057 \text{ m}^2$$

Mixing Flux: 
$$G_t = \frac{7791.7273 \frac{kg}{h.m2}}{0.0057 m^2 x 3600} = 379.189 \frac{kg}{s.m^2}$$

To  $Tm = 107 \,^{\circ}C$ , properties of the fluid are:

$$\mu = 0.00028 \ Pa.s$$
  $Cp = 3.7481 \ \frac{kJ}{kg.K}$   $k = 0.5074 \ \frac{W}{m.K}$ 

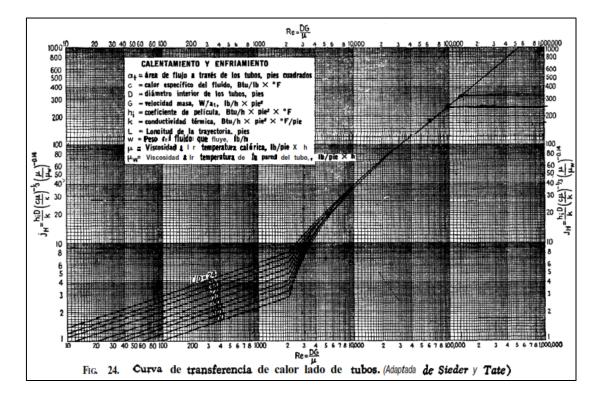
The equivalent diameter of the armor:

$$De = 4x \left( \frac{0.8661 \, x \left( \left( \left( \frac{0.0254}{0.0254} \right) \right)^2 - \frac{\pi}{4} \, x \left( \frac{0.0191}{0.0254} \right)^2 \right)}{\pi \, x \left( \frac{0.0191}{0.0254} \right)} \right) x \, 0.0254 \, = 0.01815 \, m$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{379.189 \times 0.01815 \, m}{0.00028 \, Pa. \, s} = 24953.01$$

From Fig. 24 of the book "Heat Transfer Processes" by Donald Kern, Factor Jh is extracted for the given Reynolds number:



$$Jh = 90.00$$

So:

$$Ho = Jh \ x \ \frac{k}{De} \ x \ \left(\frac{C \ \mu}{k}\right)^{1/3} = 3190.9452 \ \frac{W}{m^2. K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

For purposes of calculation, the hi recommended by Donald Kern for steam flow:

$$h_i = 8000 \frac{W}{m^2 \cdot K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{8000 \times 3190.9452}{8000 + 3190.9452} = 2281.0908 \frac{W}{m^2 \cdot K}$$

Area required for heating:

$$A1 = \frac{9280000}{3.6 \times 58.2496} = 19.4004 \ m^2$$

### E. Checking the maximum flow of heat.

Total clean area Ac:

$$Ac = A1 = 19.4004 m^2$$

• Total design coefficient:

Total area = Nt x LT x RT = 
$$86 \times 5 \times 0.1963 \frac{ft^2}{ft} \times 0.3048 m = 25.7279 m^2$$
:

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Tube surface ratio per linear foot (BWG 16)

$$U = \frac{\frac{9280000}{3.6 \times 58.2496}}{25.7279} = 172.0078 \frac{W}{m^2.K}$$

# ANNEX N°12

# **IPA Distillation Tower**

- Knowing the composition of the feed stream (F), we define the IPA as light key (LK) and water as heavy key (HK), whose compositions depend on the separation to be made. The balance of matter is obtained by obtaining:

Molar composition and molar fluxes of DISTILLATE and FUNDS								
Components	F (kmol/h)	F (kmol/h) D (kmol/h) B (kmol/h) xD xB						
Acetone	2.1429	2.1429	0.0000	0.1996	0.0000			
IPA	5.0518	5.0496	0.0022	0.4704	0.0001			
Water	26.0252	3.5426	22.4826	0.3300	0.9999			
TOTAL	33.2199	10.7350	22.4849	1.0000	1.0000			

- We determine the temperature of dew and bubble of all the currents of the tower, since they will be necessary in the design of the condenser and reboiler. The procedure to be performed is the same as the one performed in the previous design.

Bubble Point supply		Temperature (°C)		Pressure (kPa)		
It is iterated until:	$\sum (yi/\alpha) - Kr$	<i>t</i> ) - Kr 0.0000 125.90 300		125.90		00
Components	F (kmol/h)	yi	Ki	$\alpha = Ki/Kr$	yi/α	xi
Hydrogen	2.1429	0.0645	18.0659	22.70	0.0028	0.0036
Acetone	5.0518	0.1521	12.6749	15.93	0.0095	0.0120
IPA	26.0252	0.7834	0.7958	1.00	0.7834	0.9844
Water	33.2199	1.0000			0.7958	1.0000

Dew Point supply		Temperatura (°C)		Presión (kPa)				
It is iterated until:	$1/\sum \alpha.xi - Kr$	0.0000	107	107.00		07.00 300		00
Components	F (kmol/h)	xi	Ki	$\alpha = Ki/Kr$	α.xi	yi		
Hydrogen	2.1429	0.0645	4.3216	8.74	0.5636	0.2788		
Acetone	5.0518	0.1521	2.1947	4.44	0.6748	0.3338		
IPA	26.0252	0.7834	0.4946	1.00	0.7834	0.3875		
Water	33.2199	1.0000			2.0219	1.0000		

- Proceeding in the same way with the other currents you get:

CURRENT	P(kPa)	T <sub>burb</sub> (°C)	Trocio (°C)
Supply	300	107.00	125.90

Distilled	250	96.45	101.00
Money	270	130.00	129.90

We applied the ShortCut Method to determine the number of ideal dishes (Nid) for a reflux (R = 1.25Rm), the feed plate (Nf), the minimum number of plates (Nm) and minimum reflux tower. The first step is to verify if the components are distributed as initially assumed, for this the Shiras equation is applied:

$$\frac{\mathbf{x}_{JD}\mathbf{D}}{\mathbf{z}_{IF}F} = \left(\frac{\alpha_{J}-1}{\alpha_{lk}-1}\right) \frac{\mathbf{x}_{lkD}\mathbf{D}}{\mathbf{z}_{lkF}F} + \left(\frac{\alpha_{lk}-\alpha_{J}}{\alpha_{lk}-1}\right) \frac{\mathbf{x}_{hkD}\mathbf{D}}{\mathbf{z}_{hkF}F}$$

- A component will be distributed if  $0 \le xJDD / zJFF \le 1$ , therefore:

	Key cor	Tava	g (°C)			
We	assume Ki	11:	5.50			
Components	F (kmol/h)	D (kmol/h)	X <sub>JD</sub> .D/Z <sub>JF</sub> .F	¿Distribuye?		
Acetone	2.1429	2.1429	7.96	9.35	1.9319	No
IPA	5.0518	5.0496	4.27	5.01	0.9996	Si
Water	26.0252	3.5426	0.85	1.00	0.1361	Si
TOTAL	33.2199	10.7350				

Conditions				
Temperature (°C)	107.00			
HF (kJ/kmol)	-2.795E+05			
HG (kJ/kmol)	-2.398E+05			
HL (kJ/kmol)	-2.795E+05			

- We calculate the minimum backflow (Rm) using the Underwood method, for this it is necessary to determine the thermal condition of the feed mixture ("q") and the value of  $\phi$  is obtained by iterating for values among the  $\alpha$  components distributed.

$$q = \frac{H_G - H_F}{H_G - H_L}$$

$$q = \frac{-2.398 - (-2.795)}{-2.398 - (-2.795)} = 1.000$$

- The values of q and  $\varphi$  are replaced in the following equations:

Calculation of the m	inimum ref	φ =	2.7971	
To supply q=	1.0000	1 - q	0.0000	
Components	Ki	$\alpha = Ki/Kr$	$\alpha.zF/(\alpha-\phi)$	$[\alpha.xD/(\alpha-\phi)].D$
Acetone	7.96	9.35	0.0920	3.0577

IPA	4.27	5.01	0.3439	11.4194
Water	0.85	1.00	-0.4359	-1.9713
TOTAL			0.0000	12.5057

$$\frac{\sum \frac{\alpha_{J}z_{JF}F}{\alpha_{J} - \phi} = F(1 - q)}{\sum \frac{\alpha_{J}x_{JD}D}{\alpha_{J} - \phi} = D(R_{m} + 1)}$$

D(Rm+1)	12.5057
Rm	0.1649

- The minimum number of plates (Nm) is determined by the equation of Fenske:

αlkAV	5.01
R/Rm	1.25
R	0.21
$\mathbf{X} = (\mathbf{R} - \mathbf{Rm})/(\mathbf{R} + 1)$	0.03
(N-Nm)/(N+1)	0.63
Nid	15.05

$$N_{m} = \frac{\log \left[ \left( \frac{x_{lk}}{x_{hk}} \right)_{D} \left( \frac{x_{hk}}{x_{lk}} \right)_{B} \right]}{\log(\alpha_{lkAV})} - 1$$

$$\alpha_{lkAV} = \sqrt{\left(\frac{K_{lk}}{K_{hk}}\right)_D \left(\frac{K_{lk}}{K_{hk}}\right)_B}$$

The number of theoretical plates (N) for a given reflux ratio (R = 1.25Rm) is determined by the correlation of Gilliland:

$$X = \frac{R - R_{\text{m}}}{R + 1}$$

$$\frac{N - N_{m}}{N + 1} = 1 - e^{\left[\frac{1 + 54.4X}{11 + 117.2X} \left(\frac{X - 1}{X^{0.5}}\right)\right]}$$

NR/NS	0.06
NR	0.82

		NS		14.	23					
	COMPOSITION AND MOLAR FLUX OF LIQUID									
	G (kmol/s) 0.0036									
Nº	COMPONENTS	M (kg/kmol)	yi		Gi nol/h)					
1	Acetone	58.080	0.1996	2.5	5847					
2	IPA	60.090	0.4704	6.0	0907					
3	Water	18.016	0.3300	4.2	2730					
	Mavg (kg/kmol)	45.80	1.0000	12.	9484					

Kirkbride equation gives an approximate location of the supply plate:

$$\frac{N_R}{N_S} = \left[ \left( \frac{z_{hkF}}{z_{lkF}} \right) \left( \frac{x_{lkB}}{x_{hkD}} \right) \left( \frac{B}{D} \right) \right]^{0.206}$$

- For the design of perforated plates of cross-flow of a single step was taken into consideration the maximum flows of both liquid and vapor in the tower, the procedure carried out is the same as the one performed for the previous design.

- The physical properties of the fluids were obtained from the Aspen Hysys

	COMPOSITION AND MOLAR FLUX OF LIQUID											
		L (kmc	ol/s)		0.0098							
					PHY	YSICA	AL P	ROPERTIES	S OF FI	LUIDS		
CONDIT			ERATION	N (	l (K	g/KHI PG	(kg/	$m3)^{X}$	,	V(Aporo Dhinsi	ty	3.952
P (kPa)	1 P	ressureAce	tone270.0		58	O18p0.	(kg/	m <b>3</b> ),07	729	Liquat B Densi	ty	798.8
g (m/s2)	2 (	Gravity IF	A 9.807		60	<b>0</b> 99.	(kg/	m. <b>0</b> )17	720 V	isc <b>6s09</b> 3 <b>0</b> f st	eam	8.65E-06
	3	Wa	ater					n)0.75		sulla Costensi		0.047
		Mavg (kg/	/kmol)		2	8. <b>µ</b> Z	(kg/	m. <b>1)0</b> (	000V	isc <b>35143BQ</b> su	pply	2.95E-04

simulator database for each stream

defined by its composition at the bottom of the tower and at the bubble and dew point temperature.

- The following initial characteristics of the dish were taken from which the dimensions of the tower are calculated, as well as checking that there are no operational problems (flooding, whining, dragging, etc.).

PL	ATE CHARACTERISTIC	OBSERVATIONS	
do (m)	Diameter of the hole	0.0045	Tabla 6.2 - Ítem 2
p' (m)	Distance between holes	0.015	p' = (2.5 - 5).do
t (m)	Spacing Tower	0.25	Tabla 6.1 - Ítem 1

- The following preliminary calculations of flows:

$$G' = G. \overline{M}_{avgG} = 0.165 \text{ kg/s}$$

$$Q = \frac{G'}{\rho_G} = 0.04 \text{ m}^3/\text{s}$$

$$L' = L. \overline{M}_{avgL} = 0.277 \text{ kg/s}$$

$$q = \frac{L'}{\rho_I} = 3.47 \times 10^{-4} \text{ m}^3/\text{s}$$

### **Diameter of Tower (T):**

An orifice diameter of = 4.5 mm has been taken on an equilateral triangle distribution with distances p '= 15 mm between the centers of the holes.

$$\frac{A_o}{A_a} = 0.907 \left(\frac{d_o}{p'}\right)^2 = 0.0816 < 0.1$$
 (Ecuación 6.31)

From Table 6.2 - Item 1 we determine the ranges for the calculation of the constants  $\alpha$  and  $\beta$ , considering a spacing of t = 0.25 m.

$$\frac{L'}{G'} \left(\frac{\rho_G}{\rho_L}\right)^{0.5} = 0.1184$$

$$\alpha = 0.0744 t + 0.01173 = 0.0275$$

$$\beta = 0.0304 t + 0.015 = 0.0205$$

- Calculation of the flood constant (C<sub>F</sub>):

$$C_{F} = \left[\alpha \log \frac{1}{(L'/G')(\rho_{G}/\rho_{L})^{0.5}} + \beta\right] \left(\frac{\sigma}{0.020}\right)^{0.2} = 0.0547 \qquad \text{(Equation 6.30)}$$

$$V_{F} = C_{F} \left(\frac{\rho_{L} - \rho_{G}}{\rho_{G}}\right)^{1/2} = 0.78 \text{ m/s} \qquad \text{(Equation 6.29)}$$

- Using 70% of the flood speedV =  $0.70 \text{ V}_F = 0.54 \text{ m/s}$ 

$$A_n = \frac{Q}{V} = 0.077 \text{ m}^2$$

We choose a length of the spill  $W=0.80\ T$ , therefore from Table 6.1 - Item 4  $A_d=0.14145\ At$ 

$$A_n = A_t - A_d = A_t - 0.14145 At = (1 - 0.14145) A_t$$

$$A_t = \frac{A_n}{1 - 0.14145} = 0.089 \text{ m}^2$$

$$T = \sqrt{\frac{4A_t}{\pi}} = 0.338 \text{ m}$$

 We choose T ^ '= 0.50 m as the diameter of the tower and proceed to correct the total area previously calculated:

$$A_t' = \frac{\pi T'^2}{4} = 0.196 \text{ m}^2$$

$$W = 0.80 \text{ T}' = 0.4 \text{ m}$$

$$A_d = 0.14145 A_t' = 0.0278 m^2$$

- From Table 6.2 - Item 4 for a  $T' = 0.50 \, \text{m}$  we obtain  $A_a = 0.51 \, A_t' = 0.0997 \, \text{m}^2$ , therefore verifying the flow of the liquid:

$$\frac{q}{W} = 0.0009 \frac{m^3}{m.s} < 0.015 \frac{m^3}{m.s}$$
 (0. K.)

#### **Depth of Liquid (hw + h\_1):**

- We assume a height of the overflow (hW) of:

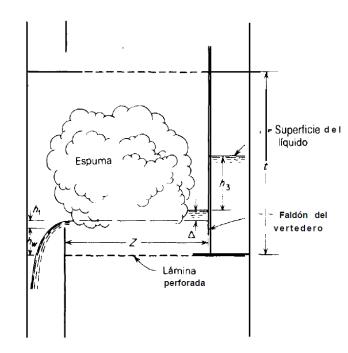
$$h_W = 50 \text{ mm}$$

- Iterate until  $h_1 = h_1'$ , para  $h_1 = 6.2$  mm in Equation 6.34:

$$\left(\frac{W_{eff}}{W}\right)^2 = \left(\frac{T}{W}\right)^2 - \left\{ \left[ \left(\frac{T}{W}\right)^2 - 1 \right]^{0.5} + \frac{2h_1}{T} \frac{T}{W} \right\}^2$$

$$W_{eff} = 0.3904 \text{ m}$$

- Replacing in Equation 6.33:



$$h_1' = 0.666 \left(\frac{q}{W}\right)^{2/3} \left(\frac{W}{W_{eff}}\right)^{2/3}$$

$$h_1' = 6.2 \text{ mm}$$

- Check the depth of the liquid:

$$h_W + h_1 = 56.2 \text{ mm} = 0.0562 \text{ m}$$

$$50 \text{ mm} < h_W + h_1 < 100 \text{ mm}$$
 (0. K.)

### Pressure Drop for Gas (hg):

- From Table 6.2 - Item 2 for a do = 4.5 mm and a stainless steel tower yields 1 / do = 0.43, therefore the orifice coefficient (Co) will be:

$$C_o = 1.09 \left(\frac{d_o}{1}\right)^{0.25} = 1.346$$
 (Equation 6.37)

- From equation  $6.31A_o/A_a = 0.0816$ , therefore  $A_o = 0.0081 \text{ m}^2$  and the gas velocity through the holes will beV<sub>o</sub> = Q/A<sub>o</sub> = 5.1 m/s.
- We calculate the Reynolds number (Re) and the Fanning friction factor (f), knowing that the absolute roughness for stainless steel is  $\varepsilon = 0.002$  mm.

$$Re = \frac{d_o. V_o. \rho_G}{\mu_G} = 10530$$

$$f = \frac{1}{4} \left\{ -1.8 \log \left[ \frac{6.9}{Re} + \left( \frac{\epsilon/d_o}{3.7} \right)^{1.11} \right] \right\}^{-2} = 0.00775$$

- Calculate the pressure drop on dry plate (hD) with Equation 6.36:

$$h_{D} = \frac{C_{o}V_{o}^{2}\rho_{G}}{2g\rho_{L}} \left[ 0.40 \left( 1.25 - \frac{A_{o}}{A_{n}} \right) + \frac{4lf}{d_{o}} + \left( 1 - \frac{A_{o}}{A_{n}} \right)^{2} \right] = 0.0113 \text{ m}$$

We determine the average flow width z = ((T + W)) / 2 = 0.450 m and the velocity based on the active area  $V_a = Q/A_a = 0.418$  m/s, therefore from Equation 6.38 we calculate the pressure drop of the liquid (hL).

$$h_L = 6.10 \times 10^{-3} + 0.725 h_W - 0.238 h_W V_a \rho_G^{0.5} + 1.225 \frac{q}{z} = 0.0334 \text{ m}$$

- The residual pressure drop (hR) is calculated from Equation 6.42:

$$h_{R} = \frac{6\sigma g_{c}}{\rho_{L}d_{o}g} = 0.0080 \text{ m}$$

- Therefore the pressure drop for the gas (hG) will be:

$$h_G = h_D + h_L + h_R = 0.0527 \text{ m}$$

$$\Delta P_G = \rho_L g h_G = 413.2 Pa$$

### **Flood Verification**

- Considering a 30 mm seal, we determine the smaller of two areas (Ada), the cross-section of the landfill (Ad) or the free area between the landfill and the plate (Afree):

$$A_d = 0.0278 \text{ m}^2$$
  $A_{free} = W(h_W - 0.03) = 0.0080 \text{ m}^2$ 

$$A_{da} = A_{free} = 0.0080 \text{ m}^2$$

- Calculate the pressure drop at the liquid inlet (h2) of Equation 6.43.

$$h_2 = \frac{3}{2g} \left(\frac{q}{A_{da}}\right)^2 = 0.0003 \text{ m}$$

- Therefore the difference in the level of the liquid inside and outside the landfill will be:

$$h_3 = h_G + h_2 = 0.0530 \text{ m}$$

- Finally verifying the flood:

$$h_W + h_1 + h_3 = 0.1092 \text{ m} < \frac{t}{2}$$
 (0. K.)

### **Whining verification**

- From Table 6.1 Item 4 for a W = 0.80 T we get Z/2 = 0.1991T, therefore Z = 0.199 m.
- We calculate the whining rate (Vow) of Equation 6.46.

$$V_{oW} = \frac{0.0229 \sigma g_c}{\mu_G} \left( \frac{{\mu_G}^2}{\sigma g_c \rho_G d_o} \frac{\rho_L}{\rho_G} \right)^{0.379} \left( \frac{l}{d_o} \right)^{0.293} \left( \frac{2 A_a d_o}{\sqrt{3} p'^3} \right)^{2.8/(Z/d_o)^{0.724}} = 3.85 \text{ m/s}$$

- whining check:

$$V_0 = 5.1 \,\text{m/s} > V_{0W}$$
 (0. K.)

### **Liquid Crawl Verification**

- To determine the drag (E) we will use Figure 6.17, for which we enter by the abscissa with the value of:

$$\frac{L'}{G'} \Big(\!\frac{\rho_G}{\rho_L}\!\Big)^{0.5} = 0.12$$

- Up to the curve  $V/V_F=0.70$ , therefore of the figure:  ${\pmb E}={\pmb 0}.{\pmb 0}{\pmb 1}{\pmb 5}$
- The drag is so small that it does not significantly modify the hydraulics of the plate.

# **Global plate efficiency**

- To determine the overall efficiency of the plate (Eo) we will use Figure 6.25, for which we enter by the abscissa with the value of:

$$\alpha_{AV}\mu_L = 1.5 \times 10^{-3}$$

- Therefore of the figure: Eo = 0.45

TOWER DISTILLATION IPA					
T (m)	Diameter of the tower	0.50			
Nr	Number of actual dishes	34			
Nf	Food dish	32			
H (m)	Tower height	8.25			
e (mm)	Wall Thickness	5			
M (kg)	Mass of cover	520			

# ANNEX N°13

# IPA Column Cap Condenser

From the following data:

Current	Inlet	Outlet	L1	L2
---------	-------	--------	----	----

Temperature (° C)	101.00	96.45	21.85	40.00
Temperature (K)	374.15	369.60	295.00	313.15
Pressure (kPa)	255.00	250.00	300.00	300.00
Fraction of vapor	1.00	0.00	0.00	0.00
Molar flow (kmol / hr)	12.9484	12.9484	393.4588	393.4588
Components				
Molar flow (kmol / hr)				
H20	4.2730	4.2730	393.4588	393.4588
IPA	6.0907	6.0907	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000
ACETONE	2.5847	2.5847	0.0000	0.0000
Molar fractions				
H20	0.3300	0.3300	1.000	1.000
IPA	0.4704	0.4704	0.000	0.000
HYDROGEN	0.0000	0.0000	0.000	0.000
ACETONE	0.1996	0.1996	0.000	0.000
Mass flow (kg / h)	593.1232	593.1232	7088.2002	7088.2002

#### A. Determination of water vapor flow.

The heat required for the condensation of the inlet flow is determined from the difference in enthalpy between the inlet and outlet conditions, for which the bubble and dew point temperature of the inlet stream was defined (T = 101 ° C and bubble T = 96.45 ° C).

$$Q_p = 474000 \frac{\text{kJ}}{\text{h}}$$

The flow rate of the cooling water (295 K):

$$\dot{m}_{water\ vapor} = \frac{474000}{66.8717} = 7088.20024 \ \frac{kg}{h}$$

#### **B.** Determination of LMTD.

$$LMTD = \frac{(374.15 \, K - 313.15 \, K) - (369.60 \, K - 295.00 \, K)}{\ln \left( \frac{(374.15 \, K - 313.15 \, K)}{(369.60 \, K - 295.00 \, K)} \right)} = 67.5721 \, K$$

#### C. Determination of the overall coefficient.

• Coefficient of heat transfer per armor - ho.

Outer tube diameter:  $D_o = 0.0191 \, m^2$ 

Separation between Pitch and Do:  $C' = 0.0064 \text{ m}^2$ 

Armor Diameter:  $D_c = 0.3874 m (15.25 pulg.)$ 

Space between baffles: B = 0.0775 m

Armored area:  $As = \frac{0.0064 \times 0.3874 \times 0.0775}{0.0254} = 0.0076 \text{ m}^2$ 

Water mass flow:  $G_t = \frac{7088.2002 \frac{kg}{h.m2}}{0.0076 m^2 x 3600} = 260.405 \frac{kg}{s.m^2}$ 

To T average =  $30.93 \,^{\circ}C$ , the properties of the cooling water are:

$$\mu = 0.00076 \, Pa.s$$

$$Cp = 4.2267 \frac{kJ}{kg.K}$$

$$k = 0.6217 \; \frac{W}{m.K}$$

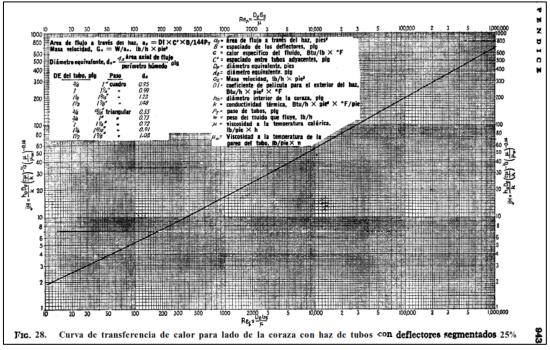
The equivalent diameter of the armor:

$$De = 4 x \left( \frac{0.8661 x \left( \left( \frac{0.0254}{0.0254} \right)^2 - \frac{\pi}{4} x \left( \frac{0.0191}{0.0254} \right)^2 \right)}{\pi x \left( \frac{0.0191}{0.0254} \right)} \right) x 0.0254 = 0.01815 m$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{260.405 \times 0.01815 \, m}{0.00076 \, Pa. \, s} = 6299.13$$

From Fig. 28 of the book "Heat Transfer Processes" by Donald Kern, Factor Jh is extracted for the given Reynolds number:



Jh = 40.00

So:

$$ho = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 6785.5673 \ \frac{W}{m^2.K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

Internal area of a tube: 
$$A_{tr} = \frac{\pi x Di^2}{4} = 0.00019 m^2$$

Pipe area: 
$$A_t = \frac{Nt \ x \ A_{tr}}{Number \ of \ steps} = \frac{122 \ x \ 0.00019}{2} = 0.01182 \ m^2$$

Mixing Flux: 
$$G_t = \frac{593.1232 \, kg/h}{0.01182 \, m^2} = 13.94 \, \frac{kg}{s.m^2}$$

To  $T_m = 96.45 \,^{\circ}C$ , the properties of the mixture are:

$$\mu = 0.000008 \ Pa.s$$

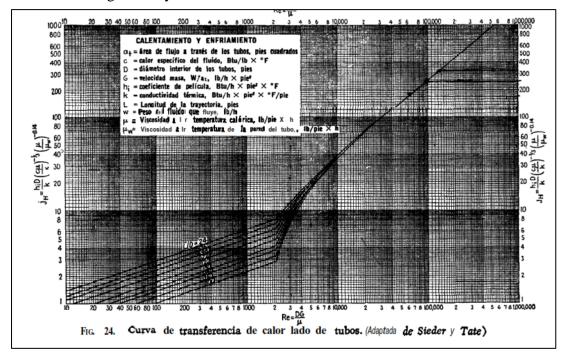
$$Cp = 1.7324 \frac{kJ}{kg.K}$$

$$k = 0.0370 \frac{W}{m.K}$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{13.94 \times 0.0157 \, m}{0.000008 \, Pa. \, s} = 25933.93$$

From Fig. 24 of the book "Heat Transfer Processes" by Donald Kern, Factor Jh is extracted for the given Reynolds number:



Jh = 160.00

Así:

$$hi = Jh \ x \ \frac{k}{De} \ x \ \left(\frac{C \ \mu}{k}\right)^{1/3} = 90.3933 \ \frac{W}{m^2. K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{6785.5673 \times 90.3933}{6785.5673 + 90.3933} = 89.2050 \frac{W}{m^2.K}$$

Area required for heating:

$$A1 = \frac{\frac{474000}{67.5721 \times 3.6}}{89.2050} = 32.9117 \ m^2$$

### D. Checking of maximum heat flow.

• Total clean area Ac:

$$Ac = A1 = 32.9117 m^2$$

• Total design coefficient:

Total area = Nt x LT x RT = 
$$122 \times 5 \times 0.1963 \frac{ft^2}{ft} \times 0.3048 m = 36.4977 m^2$$
:

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Tube surface ratio per linear foot (BWG 16)

$$UD = \frac{\frac{474000}{67.5721 \times 3.6}}{36.4977} = 53.3879 \frac{W}{m^2 \cdot K}$$

# ANNEX N°14

## IPA reflux pumps

From the following data obtained from the material balance.

Current	IPA recycle

Temperature (° C)	96.450	96.450
Pressure (kPa)	230.00	250.00
Fraction of vapor	0	0
Molar flow (kmol / hr)	2.2134	2.2134
Components		
Molar flow (kmol / hr)		
HYDROGEN	0	0
ACETONE	0.442	0.442
IPA	1.041	1.041
H20	0.7304	0.7304
Mass flow (kg / h)	101.39	101.39
Density (kg / m3)	710.5000	710.5000
Flow rate (m3 / s)	0.00004	0.00004

Performing energy balance at pump inlet and outlet:

$$E_1 + H_B = E_2$$

$$\frac{P_1}{\gamma} + Z_1 + \frac{\overline{V}_1}{2g} + H_B = \frac{P_2}{\gamma} + Z_2 + \frac{\overline{V}_2}{2g}$$

$$H_B = \frac{P_2}{\gamma} - \frac{P_1}{\gamma} = \frac{300.2 \text{ kPa}}{9.81 \text{ N x 777.6 } \frac{\text{kg}}{\text{m}^3}} = 39.354 \text{ m}$$

For the design, the data of the impeller diameter, roughness, rotational speed.

Design data	
Impeller Diameter Da (m)	0.371

Pump head H (m)	2.8694
Rotational speed n (1 / sec)	1.4
Power of pump P (W)	0.7927761
Discharge flow Q (m3 / s)	0.00004
Viscosity (Kg / m.s)	0.001
Density (Kg / m3)	710.5000
Roughness $\square$ (m)	0.0001
Coefficient of capacity Cq	0.0006
Coefficient of head Ch	104.343
Power factor CP	0.0579

# ANNEX N°15

# **Column bottom reboiler IPA**

From the following data:

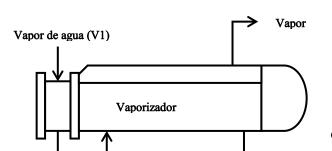
Current	В	V	V + B	V1	V2
Temperature (° C)	129.94	129.94	127.73	165.00	165.00
Temperature (K)	403.09	403.09	400.88	438.15	438.15
Pressure (bar)	270.00	270.00	275	7.00	7.00
Fraction of vapor	0.00	1.00	0.00	1.00	0.00
Molar flow (kmol / hr)	22.4849	22.4849	35.4332	166.7445	166.7445
Components					
Molar flow (kmol / hr)					
H20	22.4826	12.9483	35.4310	166.7445	166.7445
IPA	0.0022	0.0000	0.0022	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000
ACETONE	0.0000	0.0000	0.0000	0.0000	0.0000
Molar fractions					
H20	0.9999	0.9999	0.9999	1.000	1.000
IPA	0.0001	0.0001	0.0001	0.000	0.000
HYDROGEN	0.0000	0.0000	0.0000	0.000	0.000
ACETONE	0.0000	0.0000	0.0000	0.000	0.000
Mass flow (kg / h)	405.1600	233.3419	638.5019	3003.9186	3001.4008

### E. Heat balance.

For design considerations for a vaporizer, only 80% of the inlet flow to the schematic can be vaporized:

$$Vapor\ Ratio = \frac{12.9484}{35.4333} = 0.3654$$

The outline of the team is as follows:



For the determination of the overall transfer coefficient, we have the following calculation sequence:

#### F. Determination of water vapor flow.

The heat required for the vaporization of the inlet flow is:

$$Q_p = 6227000 \frac{\text{kJ}}{\text{h}}$$

The required steam flow rate (165 ° C and 700 kPa):

$$\dot{m}_{water\ vapor} = \frac{6227000}{2072.959} = 3003.9186 \ \frac{kg}{h}$$

#### G. Determination of LMTD.

Since the heating medium (water vapor) has a constant temperature profile, it is feasible to calculate the LMTD as follows:

$$LMTD = \frac{(438.15 K - 403.09 K) - (438.15 K - 400.88 K)}{\ln \left( \frac{(438.15 K - 403.09 K)}{(438.15 K - 400.88 K)} \right)} = 36.1537 K$$

#### H. Determination of the overall coefficient.

• Coefficient of heat transfer per armor - ho.

Outer tube diameter:  $D_o = 0.0191 \, m^2$ 

Separation between Pitch and Do:  $C' = 0.0064 \text{ m}^2$ 

Armor Diameter:  $D_c = 0.3366 m (15.25 pulg.)$ 

Space between baffles: B = 0.0673 m

Armored area: 
$$As = \frac{0.0064 \times 0.3366 \times 0.0673}{0.0254} = 0.0057 \text{ m}^2$$

Mixing Flux: 
$$G_t = \frac{7791.7273 \frac{kg}{h.m2}}{0.0057 m^2 x 3600} = 379.189 \frac{kg}{s.m^2}$$

To  $Tm = 129.94 \,^{\circ}C$ , the properties of the fluid are:

$$\mu = 0.00021 \, Pa. \, s$$
  $Cp = 4.2546 \, \frac{kJ}{kg.K}$   $k = 0.6878 \, \frac{W}{m.K}$ 

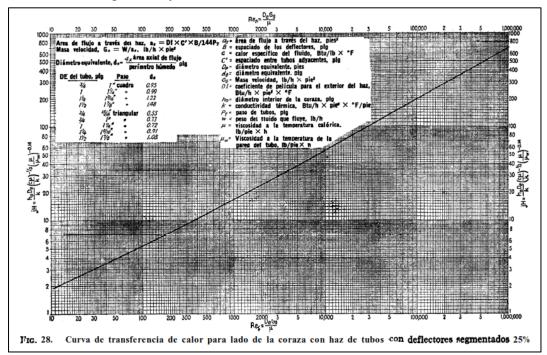
The equivalent diameter of the armor:

$$De = 4x \left( \frac{0.8661 \, x \left( \left( \left( \frac{0.0254}{0.0254} \right) \right)^2 - \frac{\pi}{4} \, x \left( \frac{0.0191}{0.0254} \right)^2 \right)}{\pi \, x \left( \frac{0.0191}{0.0254} \right)} \right) x \, 0.0254 \, = 0.01815 \, m$$

The Reynolds number is:

$$Re = \frac{G_t \times Dt}{\mu} = \frac{286.252 \times 0.01815 \, m}{0.00021 \, Pa. \, s} = 32586.36$$

From Fig. 24 of the book "Heat Transfer Processes" by Donald Kern, Factor Jh is extracted for the given Reynolds number:



$$Jh = 100.00$$

So:

$$Ho = Jh \ x \ \frac{k}{De} \ x \left(\frac{C \ \mu}{k}\right)^{1/3} = 4144.0546 \ \frac{W}{m^2. K}$$

• Determination of the coefficient of heat transfer by tubes - hi.

For purposes of calculation, the hi recommended by Donald Kern for steam flow:

$$h_i = 8000 \; \frac{W}{m^2 \; . \; K}$$

For a clean overall coefficient (U1):

$$U1 = \frac{8000 \times 4144.0546}{8000 + 4144.0546} = 2729.93 \frac{W}{m^2 \cdot K}$$

Area required for heating:

$$A1 = \frac{\frac{6227000}{36.1537 \times 3.6}}{2729.93} = 17.5256 m^2$$

### I. Checking the maximum flow of heat.

• Total clean area Ac:

$$Ac = A1 = 17.5256 m^2$$

• Total design coefficient:

Total area = Nt x LT x RT = 
$$86 \times 5 \times 0.1963 \frac{ft^2}{ft} \times 0.3048 m = 25.7279 m^2$$
:

Where:

o Nt: Number of tubes in the shell

o LT: Length of tubes

o RT: Tube surface ratio per linear foot (BWG 16)

$$U = \frac{\frac{6227000}{3.6 \times 36.1537}}{25.7279} = 1859.5989 \frac{W}{m^2 \cdot K}$$

### ANNEX N°16

## **Storage Tanks for IPA and Acetone**

- With the data of capacity, service factor and the balance of the process we determine the program of production:

Nominal Capacity (MTM / Year)	21.5
Service factor (%)	93.2%
TM IPA / TM Acetone	1.34

Production program	MTM/Año	TM/DO
<b>Production Acetone</b>	20.0	58.8
IPA Requirement	26.7	78.7

- Storage capacity is required for 14 days of raw material and finished product, for which:

Density Acetone (TM / m3)	0.791
IPA Density (TM / m3)	0.786

Inventory (days)		
Acetone	14	
IPA	14	

Storage	TM	m3
Acetone	824	1041.1
IPA	1101	1401.0

- The tanks will have the following dimensions and with this we will determine the number of tanks that are required:

Dimensions of the tank (m)		
D (diameter) 10		
H (height)	5	

Tank volume (m3)		
Total V	392.7	
V filling (80%)	314.2	

Number of tanks		
Acetone	3.31	4
IPA	4.46	5

#### **DECLARATION OF CONFIDENTIALITY**

Eng. Rafael Chero Rivas, Eng. Víctor León Choy,

Professors responsible for the course Design of Plants PI-525 / A

At the request of the students Alex Renzo Condori Llacta, Fabrizio Alexander Flores Estrada, Kevin Andrei Flores Gil, Miguel Eduardo Soto Moreno, authors of the final report titled "Design of an acetone production plant via catalytic dehydrogenation of isopropyl alcohol".

#### **DECLARE**

The confidentiality of the report in question with the effects that it derives from the terms of the corresponding instruction, which regulates the management of undergraduate studies in the Faculty of Chemical and Textile Engineering in respect of final reports, submitted Confidentiality.

Lima, December 28 2015.

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