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DESIGN OF AN EXTRACTION COLUMN (A CASE STUDY OF SEPARATION OF WATER-ACETONE-ACETIC ACID USING CHLOROFORM AS SOLVENT)

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ABSTRACT

An extraction column design for the separation of water –Acetic acid – A cetone using chloroform as solvent was carried out. The data for the design were obtained from Handbooks. The simulation of the column was done using Aspen Hysys version 8.6. The mass flowrate and composition of the extract and Raffinate phases were determined along with the theoretical and actual number of stages, column diameter, column height, stage efficiency and tray spacing. Stainless steel was used as the material of construction. Finally the results of the simulation was compared with hand calculation which showed a maximum devcation of 1.3

Keywords: Extract, Feed, Raffinate, Solvent, column, phase, stage, Diameter, Height.

INTRODUCTION

Extraction processes are widely used in chemical manufacturing technology .

The process involves the transfer of materials from one phase to another. It utilizes differences in vapor pressure or solubility. The driving force here is concentration gradient. The separation of the components of a liquid mixture by treatment with a solvent in which one or more of the desired components is preferentially soluble is known as liquid-liquid extraction, the process can be broken down into three stages as follows:

- (i) Bringing the feed mixture and the solvent into intimate contact
- (ii) Separation of the resulting two phases
- (iii) Removal and recovery of the solvent from each phase.

Extraction is in many ways complementary to distillation and is preferable in the following cases:

- (i) When distillation would require excessive amount of heat, such as for example when the relative volality is near unity.
- (ii) When the components to be separated are quite different in nature.

METHODOLOGY

Material Balance

Mass balance is written from the principle of conservation of mass and is written as :

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[Accumulation of total mass] = [inflow of total mass] - [outflow of total mass]
(1)
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But there is no accumulation of mass in the system, therefore equation (1) can be rewritten as:

[inflow of total mass] = [outflow of total mass](2)

FEED

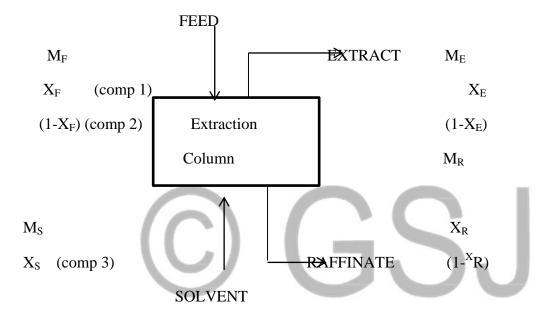


Fig 1: General schematic representation of an extraction column

Material balance of fig 1 is performed as follows:

Overall mass balance

$$M_F + M_s = M_E + M_R \tag{3}$$

Mass balance of component 1

$$M_F(X_F) = M_E(X_E) + M_R(X_R) \tag{4}$$

Mass balance of component 2

$$M_F(1 - X_F) = M_R(1 - X_R)$$
(5)

Mass balance of component 3

$$M_{S}(X_{S}) = M_{E}(1 - X_{E})$$
(6)

Where :

 M_F = mass flow rate of the feed in kg/h

 M_S = mass flow rate of the solvent in kg/h

 M_E = mass flow rate of the extract in kg/h

 M_R = mass flow rate of the raffinate in kg/h

 X_F = composition of solute in component 1

 $(1 - X_F)$ = composition of solute in component 2

 X_S = composition of solvent

 X_E = composition of solute in extract in component 1

- $(1 X_E)$ = composition of solute in extract in component 3
- $(1 X_R) =$ composition of solute in raffinate in component 2

CALCULATION PROCEDURE

Determination of theoretical number of stages

$$N = \frac{in\left[\left(\left(\frac{X_f - Y_s/m}{X_r - Y_{s/m}}\right)\left(1 - \frac{1}{\varepsilon}\right) + \frac{1}{\varepsilon}\right)\right]}{in\varepsilon}$$
(7)

Equation (7) applies only when $\varepsilon \neq 1$ if $\varepsilon = 1$ equation (7) becomes

$$N = \left(\frac{X_f - Y_{s/m}}{X_r - Y_{s/m}}\right) - 1 \tag{8}$$

Where:

N = theoretical number of stages

- X_f = solute concentration in the feed
- X_r = solute concentration in the raffinate
- Y_s = concentration of solvent
- ε = extraction factor
- M = slope of the equilibrium line

Determination of Column Diameter

$$D_c = \sqrt{\frac{4Q_c}{0.4\pi V_{cf}}} \tag{10}$$

Where:

 D_c = Column diameter

Q_c = Volumetric flow rate of the continuous phase

 V_{cf} = velocity of the continuous phase

Determination of Column Height

$$Z_c = \frac{HETS}{N}$$
(11)

S.I

Where:

 Z_c = Height of Column

HETS = Height equivalent to a theoretical stage

N = theoretical number of stages

The Height can also be computed as

$$Z_c = \frac{H_{or}}{N_{or}} \tag{12}$$

Where:

 H_{or} = Height pf a transfer unit based based on raffinate phase composition

N_{or} = Number of transfer unit

Alternatively

$$Z_c = [Actual number of stages] [Tray spacing]$$
(13)

Where

Actual number of stages =
$$\frac{theoritical number of stages}{Efficiency}$$
 (14)

SIMULATION PROCEDURE

Table 1: Operating data of feed conditions

Parameters	Value/Unit
Temperature	50° <i>C</i>
Pressure	130Kpa
Molar flow rate	1000Kgmol/h

Table 2: Feed Composition data

Component	Value
Water	0.3
Acetone	0.2
Acetic acid	0.5
chloroform	0

Table 3: solvent conditions data

Parameter	Vaule/unit
_	
Temperature	50° <i>C</i>
Pressure	130Kpa
Molar flow rate	3000Kgmol/h

 Table 4: Solvent composition data

Component		Value		
Water			0	
Acetone	()	1	0	
Acetic acid			0	
chloroform				

selection of components :

Open a new case in Aspen Hysys and select the components: Water, Acetone, Acetic acid and Chloroform as shown below.

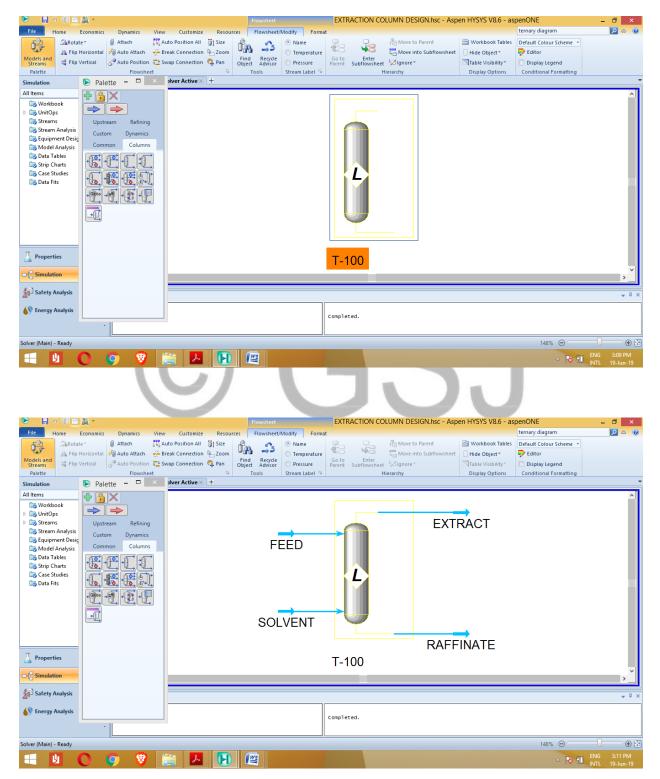
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Selection of Fluid package:

the fulid package that will be used in the simulation is UNIQUAC PR as shown below:

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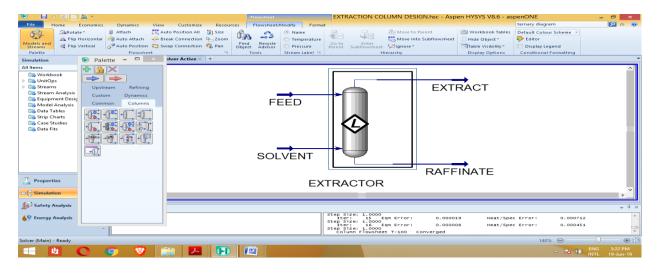
Enter the simulation environment and select the liquid-liquid extraction column and input the parameters shown in table 1



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Define the feed and solvent streams so the two streams turns blue as shown

After defining all the streams name the column Extractor and run the column which should now converge as shown



RESULT AND DISCUSSIONS

Workbook: Case (Main)

	Material Streams Fluid F					
Name		FEED	SOLVENT	EXTRACT	RAFFINATE	
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	
Temperature	(C)	50.00 *	50.00 *	49.92	50.01	
Pressure	(kPa)	130.0 *	130.0 *	130.0	130.0	
Molar Flow	(kgmole/h)	1000 *	3000 *	3733	267.1	
Mass Flow	(kg/h)	4.705e+004	3.581e+005	4.004e+005	4815	
Liquid Volume Flow	(m3/h)	48.67	239.0	282.9	4.824	
Heat Flow	(kJ/h)	-3.631e+008	-3.919e+008	-6.795e+008	-7.559e+007	

Compositions

GS

Fluid Pk<u>c</u>

Name	FEED	SOLVENT	EXTRACT	RAFFINATE
Comp Mole Frac (H2O)	0.3000 *	0.0000 *	0.0088	0.9998
Comp Mole Frac (Acetone)	0.2000 *	0.0000 *	0.0536	0.0000
Comp Mole Frac (AceticAcid)	0.5000 *	0.0000 *	0.1339	0.0001
Comp Mole Frac (Chloroform)	0.0000 *	1.0000 *	0.8037	0.0001

Fig 1: Material and compositions streams

Design	Parameters	Rating Worksheet P	erformance Flows	heet Dynamics
Perfor	mance	Feeds		
Summa	72			
Column	Profiles			
	Products			
Plots			feed	solvent
		Flow Rate (kgmole/h)	1.000000e+03	3.000000e+03
		H2O	0.3000	0.0000
		Acetone	0.2000	0.0000
		AceticAcid	0.5000	0.0000
		Chloroform	0.0000	
			0.0000	1.0000
		Chloroform	extract	raffinate
			0.0000	raffinate
		Chloroform	extract	raffinate 267.0895
		Flow Rate (kgmole/h) H2O Acetone	extract 3.732911e+03 0.0088 0.0536	raffinate 267.0895 0.0998 0.0000
		Chloroform Flow Rate (kgmole/h) H2O	extract 3.732911e+03	raffinate 267.0895 0.0998 0.0000

Fig 2: percentage recovery

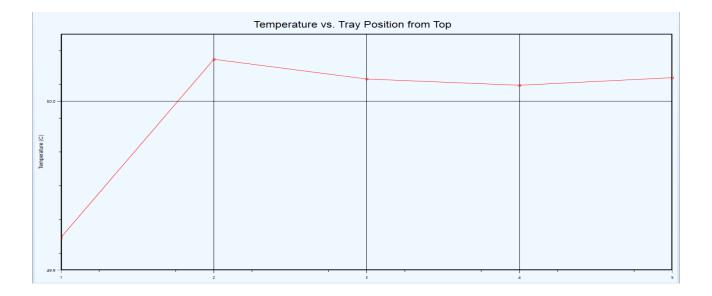


Fig 3: Temperature on each Tray from top

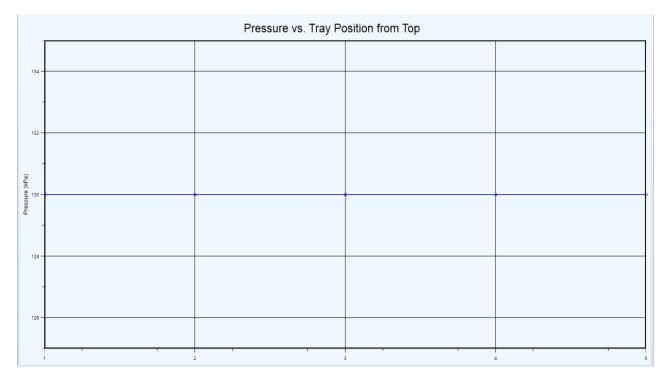


Fig 3: pressure on each tray from top

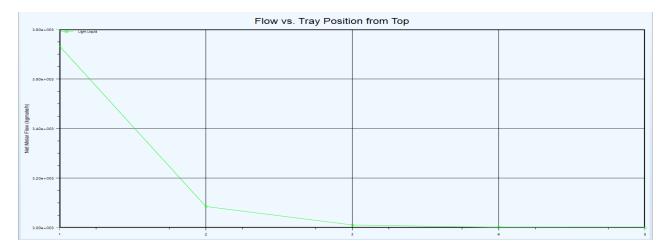


Fig 4: Molar flow rate on each tray from top

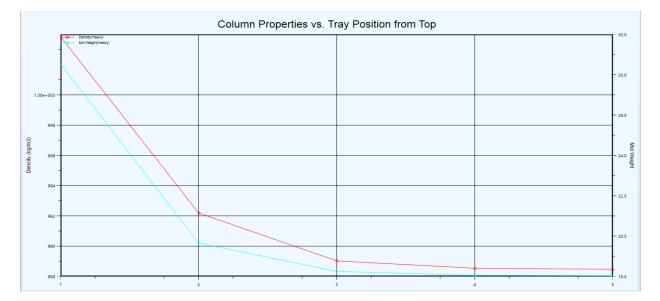


Fig 5: Density on each tray from top

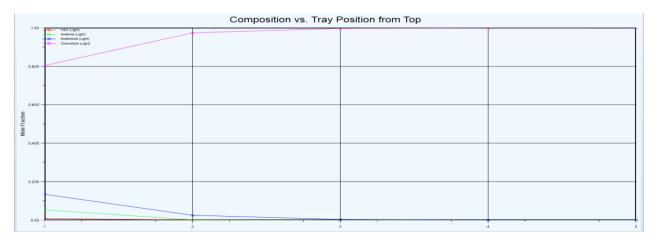


Fig 6: composition on each tray from top

The results given in the tables above reveal that although the temperature of the feed and solvent were held constant, there was a little drop in temperature in the extract phase while that of the raffinate remained constant.

There was no change in pressure in all the streams.

The molar flow rate of the extract is far greater than that of the raffinate as the solvent has extracted a large amount of the feed streams.

Acetone was completely extracted as its composition in the raffinate phase is zero.

Only a very small fraction of the Acetic acid was left in the raffinate phase.

CONCLUSION

Parameter	Calculation	Hysys	Difference
Number of theoretical stages	4.5	5	0.5
Actual number of stages	6	7	1
Stage efficiency	0.7	0.7	0
Column Diameter	1.2m	1.5m	0.3
Column Height	3m	3.5m	0.5
Tray type	sieve	sieve	
Material of construction	Stainless steel	Stainless steel	
Tray thickness	0.1mm	0.1mm	0

Table 5: Comparison between Hand Calculation and Aspen Hysys

It is observed that the less the stage efficiency the more the theoretical number of stages, hence a high stage efficiency design should be done in further research in order to reduce the number of stages for the separation.

Chloroform has a high recovery percentage for the feed mixture and should be used for large scale industrial extraction of Acetone and Acetic acid.

Acknowledgement

I wish to thank Dr. Akpa Jackson, Mrs. S.P. Oboho, Dr. K.K. Dagde, my Parents and siblings who ensured that the this work became a reality.

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