TO STUDY THE PERFORMANCE OF BATCH DISTILLATION USING gPROMS

A Thesis Submitted In
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By

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CERTIFICATE

This is to certify that the thesis entitled, “**STUDY THE PERFORMACE OF BATCH DISTILLATION USING gPROMS”** submitted by **Abdullah Saleh Awad Ba Mehrez** in fulfillment of the requirements for the award of Bachelor of Technology in **Chemical Engineering** at the National Institute of Technology, Rourkela is an authentic work carried out by him under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University/ Institute for the award of any Degree or Diploma.

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ABSTRACT

The detailed dynamic modelling,and simulation of a batch distillation process is presented. The model considers a mixture of 5 components separated in a 20 tray column. Simulations performed in the process modelling tool gPROMS proved that the model gives a very accurate description of the process behaviour. Overall, gPROMS proved to be a powerful tool for solving problems of large scale models of great complexity such as the batch distillation process. One of the reasons for this is its ability to model and handle discontinuities of the types that very often occurs in chemical processes (for example, when changing the reflux ratio during a distillation operation). As with any other chemical process, the modelling of batch distillation requires the accurate consideration of physical properties in order to model the thermodynamics of the process in an accurate manner.

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1. Introduction

1.1 Background

One of the major operations in the chemical and pharmaceutical industries is the separation of liquid mixtures into their components using distillation. The distillation can be performed as either a continuous or a batch process. Batch distillation has several advantages in many cases and it is often used in industries where high purity products are produced. In particular, it is used for purifying products or recovering solvents or valuable reactants from waste streams. Batch distillation has the advantage of being much more flexible than continuous distillation, as it has more degrees of freedom (e.g. flow rate, temperature, pressure). The flexibility makes it possible to cope with varying compositions of feed and product specifications; also completely different mixtures can be separated using the same column. This is a big advantage with today's frequently changing product specification requirements of the market (Galindez and Fredenslund [1]). Furthermore batch distillation often means simpler operation and lower capital cost than continuous distillation (Skogestad, Wittgens and Sørensen [2]).

The most obvious disadvantage of batch distillation is the high cost of energy, as it most often requires more energy than continuous distillation.

The fact that the use of batch distillation as well as the competitiveness in industry has increased during the last years (Furlonge [3]) makes it interesting to model the process and to use this model for optimization, minimizing energy requirements (which, in practice, often means minimizing production time) and loss of product, always maintaining high purity requirements.

Further motivation is provided by the increasingly stringent environmental regulations, which make effective control of processes vital (Barolo [4]).

1.2 Problem Statement

As batch distillation is an inherently complex dynamic process (the holdup and composition of material change with time during operation) and as the model size of batch distillation quickly grows with increasing model accuracy, number of components and number of trays (in cases of tray columns), successful modeling and simulation relies on today’s fast development of computer hardware and software.

2. Process Description

2.1 Components

The objective of the process considered is to produce C_{10} .More specifically, starting with a feed mixture of 5 components with an initial concentration of C_{10} of about 66%.

2.2 The Column

Both a tray and a packed column are used for the separation of the mixture described above. Because of time limitation only the tray column has been considered in this work. The tray column which is used to perform the desired separation consists of 20 trays. Each tray has and the column is about 13.5 meters high with a diameter of 1 meter.

2.3 Operation Procedure

For the purposes of this thesis, the duration of the process is normalized, with 100% corresponding to 100 hours of nominal operation. The pressure difference used to regulate the production is also normalized.

2.3.1 Reflux Ratio

The operating policy used is a piecewise *constant reflux ratio*, i.e. the reflux ratio is fixed at a pre-defined value during the different time intervals of the process. This causes the distillate composition to change during the operation, as the composition of the mixture in the reboiler changes.

The operating schedule of the reflux ratio consists of five different cuts:

1. Light component off-cut:

The light components are evacuated. This takes 7 hours with the reflux ratio, R=5.

2. Off-cut:

A lighter component (C_4) in the mixture is removed without specification. The duration of this cut is 14 hours with reflux ratio R=5.

3. Intermediate cut:

The mass fraction of C_{10} should reach highest by the end of this phase. This is achieved by using a reflux ratio of 10 over 16 hours.

4. Main cut:

It is the mass fraction of C_{10} in the product accumulator. The reflux ratio is kept at 5 over 7 hours, and is then switched to 8 for an additional 54 hours.

The whole operation takes 100 hours.

2.3.2 Pressure

In addition to the reflux ratio, the pressure difference in the column (measured between reboiler and condenser) is also used as a control variable for regulating the column operation. The steam to the reboiler is controlled manually. When the pressure difference in the column is too small, the steam flow is increased by the process operator. At the top of the column, the pressure is controlled with a vacuum pump. The pressure difference in the column should measure between 0.8 and 1 bar.

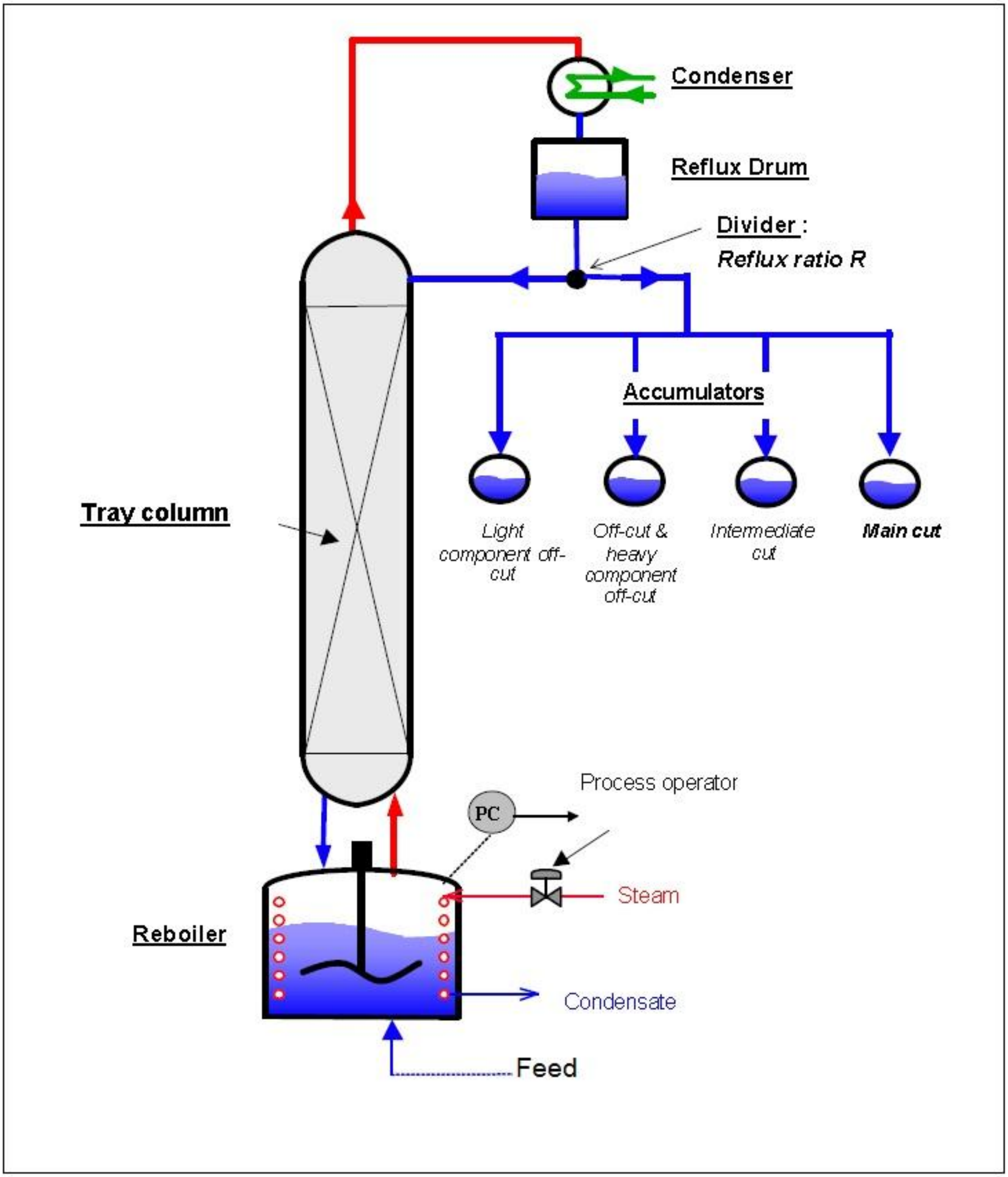

Figure 2.1 the batch distillation column.

3. The Model of the Process

3.1 Model Accuracy

In general, increased model accuracy comes at the expense of increased model complexity and decreased computational efficiency. This means that the size of the models used in practice has to be a compromise between accuracy and simplicity to avoid numerical problem and to retain computational efficiency.

The so-called “short-cut” models for batch distillation have been very widely used in the literature. Short-cut techniques develop a direct relationship between the composition in the reboiler drum and the distillate, thus avoiding the modeling of individual trays. This leads to a significant reduction in model size. This further means that the computational effort is reduced, which was of crucial importance before today’s powerful computer hardware became available (Diwekar [5]).

Much research on batch distillation has also been done using models built up by several simplified sub models, with common assumptions such as constant liquid holdup on the tray, negligible vapor holdup, constant molar overflow (neglecting the energy balance and liquid hydraulics on each tray) and ideal equilibrium stages. Some of the assumptions can, however, cause the models to give answers far from the truth (Furlonge [6]). The usefulness of the models is reduced, potentially leading to inaccurate decisions concerning operation or design, if the knowledge of the assumptions is not good enough (Nilsson [7]).

In the case of batch distillation, the problem of model mismatch is aggravated by the “integrating” nature of the batch process. Structural or parametric errors in the model cause the error in predicted composition to increase in magnitude throughout the duration of a simulated batch run. This is fundamental to the process, and is true for any model solution technique (Bosley [8])

With the latest computational capacity currently available at hand, it was possible to make use of a process model that is more detailed than most other models used for similar purposes.

3.2 The Structure of the Model

The model consists of seven different units:

- Tray
- Reboiler drum
- PI-controller
- Condenser
- Reflux drum
- Divider
- Accumulator

Each unit type is modeled separately. Then, one or more instances of each unit type are linked together to constitute the model of the whole process. This decomposition approach provides a better overview of the problem, greatly facilitating model development.

Moreover, the constructed model is more flexible than if would be the case had it been written as a single large unit.

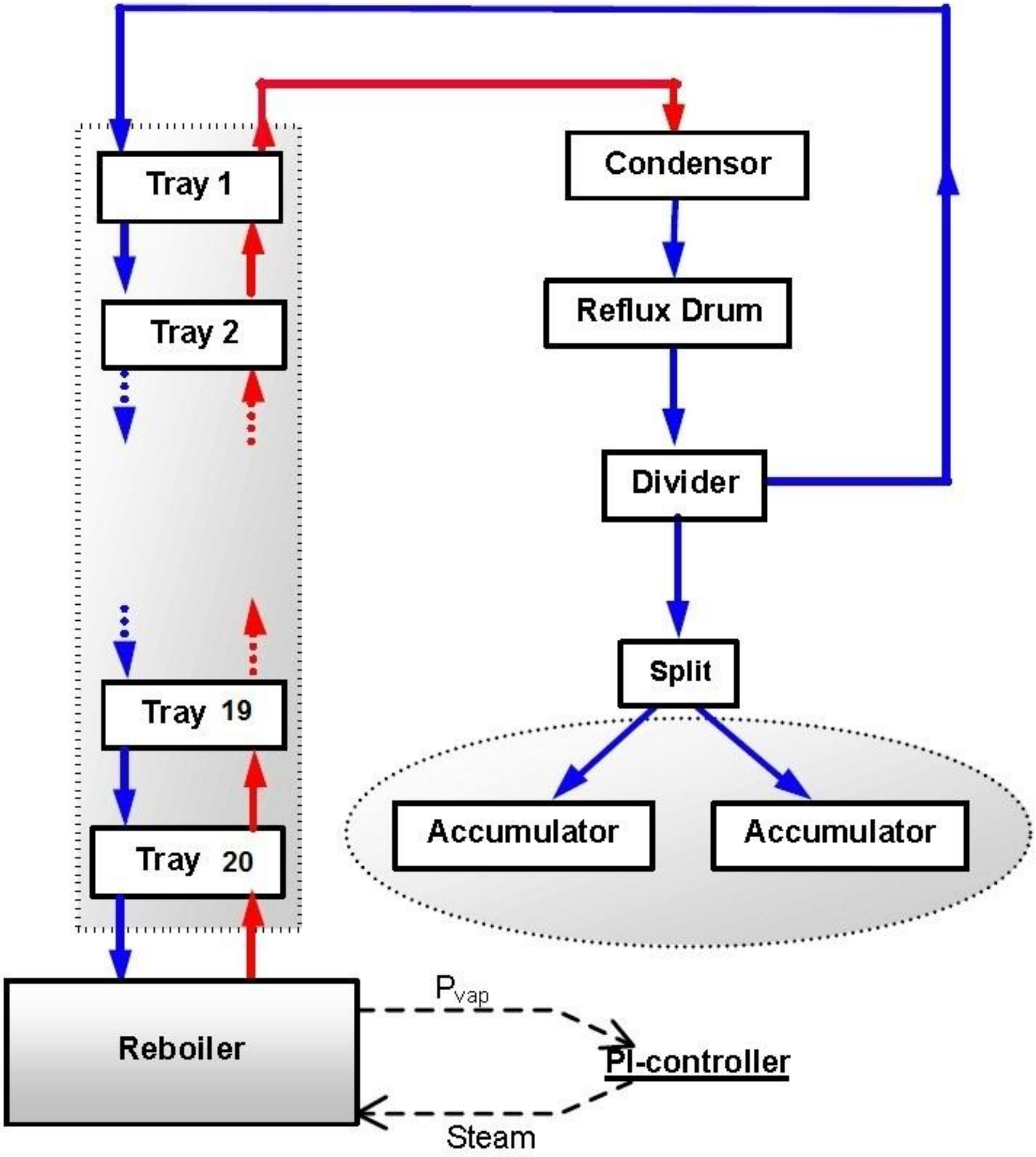

Figure 3.1 Flow sheet

The model used considers differential mass and energy balances, liquid non-ideality, and liquid hydrodynamics, with the liquid flow rate being calculated using the Francis weir formula (Perry [9]). The influence of the holdup and pressure on every tray is also taken into account.

3.3 Model Assumptions

The model for the batch distillation column has been developed using a number of model assumptions (Gautheron [10]). The final model consists of about 4000 variables/equations. The model assumptions are listed below:

1. Total condensation with no sub-cooling in the condenser.
2. No entrainment and weeping effects.
3. Constant tray efficiency.
4. Adiabatic operation.
5. Phase equilibrium.
6. Perfect mixing on the trays and in the reboiler drum.
7. Ideal vapor phase

4. gPROMS

4.1 Features of *gPROMS*

gPROMS (**g**eneral **PRO**cess **M**odeling **S**ystem) process modeling software tool that is well suited for the dynamic modeling, simulation and optimization of chemical processes. One of the reasons for this is its ability to model and handle discontinuities of the types that very often occurs in chemical processes (for example, when changing the reflux ratio during a distillation operation).

gPROMS distinguishes three fundamental types of modeling entity. `MODEL`s describe the chemical and physical behavior of the system, defined by the equations that have been specified by the user, while TASKs are descriptions of the external actions and disturbances imposed on the system. Especially when dealing with batch processes, the modeling of operating procedures is of great importance. Such operating procedures are very easily described as TASK entities, as the gPROMS TASK language provides a large variety of features, with actions being executed in sequence or in parallel, conditionally or iteratively, thus describing the operation of the process in a very general and flexible way. The third type of entity is the `PROCESS`, which is formed by a TASK driving a MODEL with some additional information, such as initial conditions and the time variation of the input variables. Thus, a simulation is defined as the execution of such a PROCESS.

As with any other chemical process, the modeling of batch distillation requires the accurate consideration of physical properties in order to model the thermodynamics of the process in an accurate manner. This work has made use of the IKCAPE physical properties package for this purpose. This package has been interfaced to gPROMS via the gPROMS Foreign Object Interface (gPROMS Introductory User Guide [11]).

Version 1.7 of gPROMS was used throughout this study.

5. Simulation of the Batch Distillation Column

A simulation of the column was performed to compare the profiles with the results from the simulation performed in SPEEDUP and furthermore to evaluate the performance of *gPROMS* during simulation.

5.1 Operating Procedure

- The light off-cut, was simulated for a period 7 h instead of 5 h, with a reflux ratio of 5 instead of 1.
- The heavy component off-cut was neglected.
- The pressure difference in the column was held constant at 1 bar during the whole simulation.

Operating procedure of the simulation:-

	Reflux ratio	Duration (in hours)
Light off-cut	5	7
Off-cut	5	14
Intermediate cut	10	16
Main cut	5	7
Main cut	8	54

Table 5.1 Operating procedure during simulation.

The total simulated operating time was thus 98 h.

5.2 Initialization

For the initialization, the column trays are assumed to contain only the light components of the mixture, whereas all the other components are charged to the reboiler. All the initial conditions given in the gPROMS file can be found in table 5.2.

To provide all the other variables of the equation system with reasonable initial guesses, a saved file from a former simulation was restored in the `PRESET` section of the gPROMS file.

Tray(i)	Reboiler	Accumualtor1 and 2	Accumulator 3	Accumulator 4	Reflux Drum	PI-controller
x(1) = 1.0	x(1) = 0.00066	x(1) = 1.0	x(1) = 0.01	x(1) = 0.01	dM_i/dt = 0.0	Error = 0.0
x(2) = 0.0	x(2) = 0.00147	x(2) = 0.0	x(2) = 0.0	x(2) = 0.0	dM/dt = 0.0	
x(3) = 0.0	x(3) = 0.149	x(3) = 0.0	x(3) = 0.0	x(3) = 0.0	dU/dt = 0.0	
x(4) = 0.0	x(4) = 0.663	x(4) = 0.0	x(4) = 0.06	x(4) = 0.0		
x(5) = 0.0	x(5) = 0.007031	x(5) = 0.0	x(5) = 0.91	x(5) = 0.98		
dM/dt = 0.0	Level = 1.0	M = 0.01	M = 0.01	M = 0.01		
dU/dt = 0.0	dU/dt = 0.0					

Table 5.2 the initialization conditions for simulation.

5.3 Simulation of the Model

The simulation of the model is simulated in gPROMS with 5 components and 20 trays with these components and their and mass fractions

Component	Mass fraction
C_1	0.13
C_4	9.75
C_{10}	66.75
C_{14}	1.32
C_{22}	22.02

Table 5.3 Feed compositions for the model.

During the simulation of the light off-cut of the case the reflux ratio was set to 3 (R = 3 was the reflux ratio used during the simulation of the light off-cut).

The composition (mass fraction) profiles obtained in the divider and the reflux ratio variation are shown below:

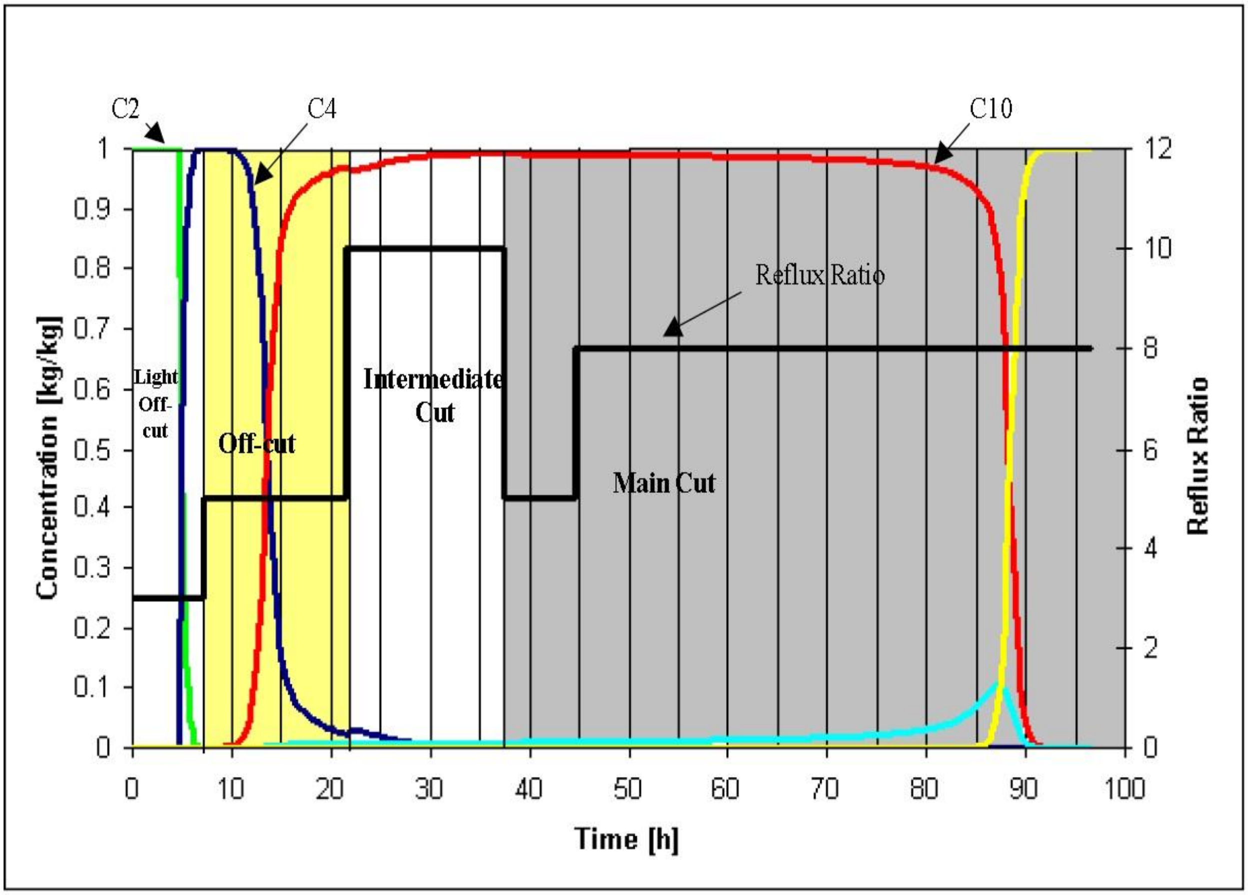

Figure 5.3 Reflux ratio and divider mass fraction profiles of the batch distillation.

6. Result and conclusion

6.1 Results

The result of the simulation and modeling of batch distillation obtained and a graph was drawn for the Reflux ratio and divider mass fraction profiles of the batch distillation.

The separation was carried away in the batch distillation where we got our three cut the light off cut, the off-cut the intermediate cut and the main cut.

This table shows the performance of batch distillation in separating the components of the feed.

Time (hrs.)	C_2 concentration	C_4 concentration	C_{10} concentration
0	0.9999	0	0
5	0.97565	0.73456	0
10	0	0.97675	0.00121
15	0	0.12345	0.7456
20	0	0.00023	0.9546
25	0	0.000013	0.9665
30	0	0	0.9699
35	0	0	0.9711
40	0	0	0.9745
45	0	0	0.9820
50	0	0	0.9811
55	0	0	0.9780
60	0	0	0.9730
65	0	0	0.9710
70	0	0	0.9690
75	0	0	0.9650
80	0	0	0.9620
85	0	0	0.9320
90	0	0	0.00897
95	0	0	0

Table 6.1 component concentration and time taken for separation.

6.2 Validity of Model

The following experimental data was used as a basis for checking the validity of the model in gPROMS with methanol mixtures have been made with heat duties of 466.7 W, the column has worked at a constant reflux ratio 1, 1.5, 2, 2.5, and 3 respectively. The initial volume of the mixture was 4 l and all the mixtures methanol-water have the same initial composition 20% mole methanol and 80% mole of water. The column works at atmospheric pressure with 15 trays. In all the experiments the distillation still was charged and heated up under total reflux until steady-state conditions were achieved. After, the reflux ratio was turned from infinity to finite reflux ratio and product was withdrawn at the top of the column. During the column operations, the concentration profile of the liquid phase along the column. The value of experimental is depicted in table (6.2.1). The experiment depicted values of percentage mole of pure methanol in the distillate for a variation in reflux ratio, time and distillate flow rate (A.Bonsfills, L.Puigajaner [12]).

Reflux Ratio	Time of Experiment	Distillate Flow rate (in mol/min)	% mole of pure methanol recovered in the distillate
1	5 h 15 min	0.23	46.8
1.5	5 h 30 min	0.20	48.8
2	5 h 45 min	0.17	50.7
2.5	6 h	0.16	56.4
3	6 h 30 min	0.15	59.1

Table 6.2.1 the value of experimental batch distillation

The same parameters which were used in the experiment were incorporated in the gPROMS model. The results of the percentage mole of pure methanol recovered in the distillate were then estimated. The estimated values using the gPROMS model are presented in table (6.2.2).

Reflux Ratio	Time of Experiment	Distillate Flow rate (in mol/min)	% mole of pure methanol recovered in the distillate	Error Percentage between experimental and simulated results
1	5 h 15 min	0.23	48.3	3.2
1.5	5 h 30 min	0.20	51.1	4.7
2	5 h 45 min	0.17	54.6	7.7
2.5	6 h	0.16	59.7	5.9
3	6 h 30 min	0.15	64.5	9.1

Table 6.2.2 the estimated values using the gPROMS model for the batch distillation

The table (6.2.2) represents the amount of error deviation between the experimental and the simulated results for the same set of parameters.

It is evident that the amount of estimated purity of methanol in the distillate increases with the increase in reflux ration and also the time of the experiment. This may be due to the reason that the reflux is used in large quantities to increase the vapor and liquid interaction to enhance purity. However, the distillate flow is reduced in the process. The other reasons for the expected value of purity to be greater are because of the assumptions of the model. The model assumes a constant tray efficiency which might not be the case practically. The same reason of ideality may not be found in perfect mixing on the trays and phase equilibrium assumptions too.

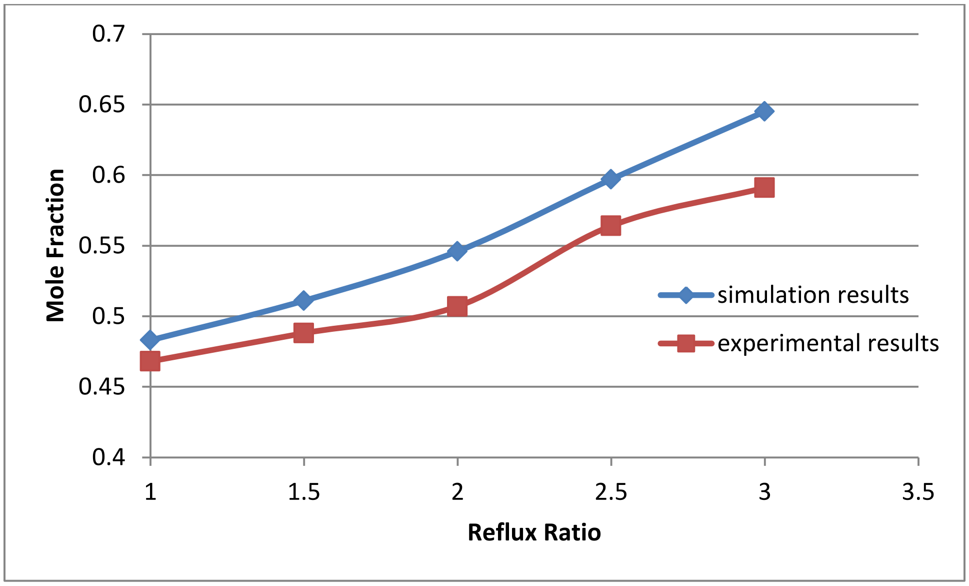

Figure 6.2 Graph of Mole fraction of methanol vs. Reflux Ratio

However, when considered for other aspects the model serves precisely. As represented in the figure (6.2), there is an error varying from 3% to 9% in the purity of the methanol in the distillate. This experimental verification thus helps in an efficient validation of the model.

6.3 Conclusion

It was found that gPROMS is a very strong software for solving complex problems like batch distillation, solving big no. of equations with big no. of variables in small time period and with a variable reflux ratio.

The concentration of the components vs. the time taken for the process of batch distillation and vs. the reflux ratio was drawn.

It was noticed due to high amount of C_{10} in the feed it was the main cut that took most of the time for separating it due its high percentage so it took most of the distillation time with high reflux ratio.

The model is valid for a batch distillation process, which was verified by experimental values owing to a maximum error of about 9%.

Nomenclature

A	Antoine’s coefficient	
Area	cross sectional area	m^2
B	Antoine’s coefficient	
bias	steady state control value	
C	Antoine’s coefficient	
C_p	heat capacity	kJ/(kmol.K)
Error	set point and variable error	
f	fugacity	
g	acceleration due to gravity	m/s^2
gain	controller gain	
h	specific enthalpy	kJ/kmol
ΔH°_{298}	latent heat of vaporisation	kJ/kmol
ΔHV298	heat of vaporisation	kJ/kmol
height	liquid level in reflux drum	m
h_f	liquid level on tray	m
h_{weir}	weir height	m
$h_{'weir}$	height of liquid above weir	m
I_{error}	integral error	
I_{in}	input signal	
k	equilibrium coefficient	
$k^{'}$	heat transfer coefficient	$W/m^2.K$
L	liquid flowrate	kmol/h
Level	liquid level in reboiler	m/m

I_w	weir length	m
M	molar holdup	kmol
MW	molecular weight	kmol/kg
N_C	number of components	
P	pressure	bar
p°	vapor pressure of pure component	Pa
ΔP	pressure drop	mbar
ΔP_{tr}	dry pressure drop	mbar
Q	rate of heat transfer	W
R	reflux ratio	
reset	reset time of PI-controller	
Sp	set point of PI-controller	
T	temperature	°C
U	internal energy	kJ
v	molar volume	m^3/kmol
$V_{downcomer}$	volume of down comer	m^3
v_f	liquid load	$m^3/(m^2.h)$
value	calculated value of PI-controller	
Vges	volume reboiler	m^3
W	mass holdup	kg
w_g	vapor velocity	m/s
x	liquid composition	kmol/kmol
x_M	liquid composition	kg/kg
y	vapor composition	kmol/kmol

F_{fac}	vapor load (F-factor)	
Greek Letters		
ε_l	Liquid fraction	
Φ	Fugacity coefficient	
γ	Activity coefficient	
η	Tray efficiency	
λ	Constant	
μ	Parameter of control variable	
ρ	Density	kg/m^3
Subscripts		
B	batch	
C	condenser	
F	feed	
I	intermediate cut	
i	component	
in	inlet	
k	tray	
out	outlet	
R	reboiler drum	
crit	critical point	
Superscripts		
L	liquid	
V	vapor	
*	Ideal composition	

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Appendix A

The Equations of the Model

A.1 Tray

Molar balance on component i:

$dM_{i,k}/dt = x_{i,k-1} \cdot L_{k-1} + y_{i,k+1} \cdot V_{k+1} - x_{i,k} \cdot L_k - y_{i,k} \cdot V_k i = 1,..N_C$

Energy balance:

$dU_k/dt = h^L_{k-1} \cdot L_{k-1} + h^V_{k+1} \cdot V_{k+1} - h^L_k \cdot L_k - h^V_k \cdot V_k$

Liquid and vapor contributions to component holdup:

$M_{i,k} = x_{i,k} \cdot M^L_k + y_{i,k} \cdot M^V_k \qquad i = 1,..N_C$

Liquid and vapor contributions to total internal energy:

$U_k = h^L_k \cdot M^L_k + h^V_k \cdot M^V_k - P_k \cdot v_k$

Equilibrium relationship:

$y_{i,k} = \eta \cdot k_i \cdot x_i + (1 - \eta) \cdot y_{i,k-1}$

Normalization equations:

$$\sum_{i=1}^{N_C} x_{i,k} = \sum_{i=1}^{N_C} y_{i,k}$$

Ideal mixing:

$x_{i,k} = x_{i,k-1}$

Liquid holdup on the tray:

$M^L{}_k = (Area \cdot h^{'}{}_{weir} \cdot \varepsilon_1 + V_{downcomer}) \cdot \rho_{liq} / MW_{liq}$

Liquid and vapour load:

$v_f \cdot l_w \cdot \rho_{liq} = 10 \cdot L_k \cdot MW_{liq}$

$w_g \cdot \rho_{vap} \cdot Area = V_{k+1} \cdot MW_{vap}$

Pressure drop across tray:

$\Delta P = \rho_{vap} \cdot g \cdot h_f + \Delta P_{tr}$

$\Delta P_{tr} = f(F_{Fak})$

A.2Reboiler Drum

Molar balance on component i:

$dM_{i,r}/dt = x_{i,R}^{in} \cdot L_R^{in} - y_{i,R}^{out} \cdot V_R^{out}$ $\qquad i = 1,..N_C$

Energy balance:

$dU_R/dt = h_R^{in} \cdot h_R^{in} - y_R^{out} \cdot h_R^{out} + Q_R$

Liquid and vapor contributions to component holdup:

$M_{i,R} = x_{i,R} \cdot M_R^L + y_{i,R}^{out} \cdot M_R^V$ $\qquad i = 1,..N_C$

Equilibrium relationship:

$y_i = k_i \cdot x_i$

Normalization equation:

$\sum y_i = 1$

Heat conduction:

$Heat = 0.0001 \cdot k' \cdot (A_{pipe} \cdot Level + A_{pipe,bottom}) \cdot (T_{steam} - T_{liq})$

T_{steam} = a. log (Steam pressure) + b

where a and b are constants.

A.3 PI-controller

$Error = Sp - I_{in}$

$d(I_{error})/dt = Error$

$value = bias + gain \cdot (error + I_{error}/reset)$

A.4 Condenser

Molar balance on component i:

$y_{i,c} = x_{i,c}$ $\qquad i = 1,..N_C$

Molar balance:

$V_C^{in} = L_C^{out}$

Energy balance:

$h_1^V \cdot V_C^{in} = h_C^L \cdot L_C^{out} + Q_C$

Equilibrium relationship:

$y_{i,out} = x_{i,out} \cdot k_i$

Normalization equation:

$\sum y_{i,out} = 1$

A.5 Reflux Drum

Molar balance on component i:

$dM_{i,k}/dt = x_{i,in} \cdot L_{in} - x_{i,out} \cdot L_{out}$ $\qquad i = 1,..N_C$

Energy balance:

$dU/dt = h_{in}^L \cdot L_{in} - h_{out}^L \cdot L_{out}$

Liquid holdup:

$L_{out} = k_{liq} \cdot height^{1.5}$

$M \cdot MW_{liq} = Area \cdot Height \, . \, \rho_{liq}$

A.6 Divider

Mass balance:

$L_{in} = L_{out,1} + L_{out,2}$

$L_{out,1} = L_{in} \cdot R$

Enthalpy balance:

$h_{out,1}^L = h_{in}^L \cdot R$

$h_{out,2}^L = h_{in}^L \cdot (1 - R) / R$

Equilibrium relationship:

$x_{in} = x_{out,1} = x_{out,2}$

Pressure:

$P^L_{in} = P^L_{out,1} = P^L_{out.2}$

Temperature:

$T^L_{in} = T^L_{out,1} = T^L_{out.2}$

A.7 Accumulator

Molar balance on component i:

$dM_i/dt = x_{in,i} \cdot L_{in}$ $i = 1,....N_C$

Liquid Volume:

$\text{Volume} \cdot \rho_{liq} = M \cdot MW_{liq}$

Conversion to mass units:

$W_i = MW_{liq,i} \cdot M_i$ $i = 1,..N_C$

$x_{M,I} = W_i / \sum_{i=1}^{N_C} W_i$

A.8 Equilibrium and Physical Properties Calculations

Equilibrium between the vapor and liquid phase is reached when the pressure, the temperature and the chemical potential of every component and the chemical potential of every component in both phases are the same. The equilibrium can be calculated by use of the fugacities, which will be equal in both phases at equilibrium:

$f_i^L = f_i^V$

This leads to:

- at low pressure: $f_i^\circ = p_i^\circ$
- ideal vapor phase: $\Phi_i = 1$
- ideal liquid phase: $\gamma_i = 1$

The separation in most separation columns used in chemical industries are operated at relative low pressure and the vapor phase can therefore be assumed to be ideal. This leads to the expression:

$$k_i = \frac{y_i^*}{x_i} = \frac{\overset{\circ}{p_i}}{p} \cdot \gamma i$$

where the vapor pressure of every pure component, $\overset{\circ}{p_i}$ is calculated with the Antoine equation:

$$\ln \overset{\circ}{p_i} = A_i + \frac{B_i}{C_i + T}$$

(the parameters A_i, B_i, C_i can be found in the literature).

The activity coefficient, γ_i depends on both the temperature and concentration of the component and can be calculated with NRTL, UNIQUAC or UNIFAC models (Anna Klingberg [13]).

Tray efficiency:

A theoretical tray means that vapor leaving the tray is in equilibrium with the liquid leaving the tray. In practice this never happens and tray efficiencies have to be used:

$$\eta_k = \frac{y_{i,k} - y_{i,k+1}}{y_{i,k}^* - y_{i,k+1}}$$

η_k is dependent of the volatility of the component and the efficiency of the mixing. η_k usually has a value between 0.7-1.0 and can easily be evaluated with an experiment. The tray efficiencies in this work have been assumed to be equal for all the components, although this is in reality only true for binary systems (Kooijman, H.A. and R. Taylor [14]).

Capacity of the column:

The capacity of a separation column is often defined as the higher limit of the steam load. The steam load is limited by the diameter of the column, the tray structure and the characteristics of the mixture to be separated. If the steam load is too small the liquid will start leaking through perforations. This phenomenon is called weeping. If the steam load is too high on the other hand, it will cause the liquid to be entrained in the vapor up the column, causing flooding. The steam load effects the tray efficiencies in a great extent.

The load factor, F-factor is defined:

$F_{Fak} = w_g \cdot \rho^{1/2}_{vap}$

Enthalpy:

Enthalpies needed for the energy balances can be calculated with:

$h_i^V = \Delta H°_{298} + \int_{298}^{T} C_{p_i}\, dT$

$h_i^L = h_i^V - \Delta HV_i^{298}$

The heat capacity, C_p and the heat of vaporization depends on temperature and can be calculated with the following correlations:

$C_{pi} = a_{i.0} + a_{i,1} \cdot T + a_{i,2} \cdot T_j^2 + a_{i,3} \cdot T_j^3$

$\Delta HV_i = \Delta H\ (T_i^v)\ (\frac{1 - T/T_{crit,i}}{1 - T_i^v/T_{crit,i}})^{0.38}$

The specific latent heat of vaporization, $\Delta H°_{298}$ can be found in literature.