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Case Report

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Comparison of Hand Calculations and ChemSep Simulation for Ethanol-Water Distillation Column Design

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Abstract

This study presents the design and simulation of a distillation column aimed at separating a binary ethanol-water mixture, using both hand calculations and ChemSep simulation. The analysis follows principles illustrated in the distillation of benzene-toluene systems and applies them to ethanol-water separation under atmospheric pressure. The column setup includes a total condenser, kettle-type reboiler, and 15 theoretical stages, with the feed being partially vaporized. Key design parameters such as reflux ratio, theoretical stages, tray efficiency, column height, and diameter were estimated using mass balances and vapor-liquid equilibrium (VLE) data. These hand calculations were compared with detailed ChemSep simulations, which incorporated the Wilson thermodynamic model for improved accuracy. While the manual approach assumed constant relative volatility and simplified energy balances, the simulation provided refined results through dynamic VLE modeling and enthalpy data. The comparison highlighted variations in tray count, column sizing, and energy use, emphasizing the importance of simulation tools in process design. The study concludes with practical insights into industrial applications, material selection, and a cost estimate for constructing a lab-scale distillation unit.

Keywords: Distillation, Ethanol-Water Separation, ChemSep Simulation, Reflux Ratio, Relative Volatility, McCabe-Thiele, Tray Efficiency, Column Design, Mass Balance, Vapor-Liquid Equilibrium

1. Problem Statement

This study focuses on the design and simulation of a distillation column for separating a binary mixture of ethanol and water. The process is based on Example 5.17 from K.V. Narayanan and B. Lakshmikutty's "Mass Transfer, Theory and Applications", which details the separation of a benzene-toluene solution in a plate column with 15 stages, a total condenser, and a kettle-type reboiler. In our case, the objective is to separate an ethanol-water mixture using a similar setup, ensuring the desired separation is achieved with optimized energy efficiency. The column operates at 101.3 kPa, and the feed is partially vapourized, with one-third in the vapour phase and two-thirds in the liquid phase. To match the desired production scale, the feed flowrate was adjusted to obtain 100 kg/day of the final product.

1.1 Introduction to the Distillation Process

Distillation is a widely used separation technique in chemical industries, particularly for the purification of liquid mixtures based on differences in volatility. The ethanol-water distillation process follows fundamental mass and energy balance principles, utilizing vapour-liquid equilibrium (VLE) data for design calculations. The separation is achieved through a plate column equipped with a total condenser and a kettle-type reboiler, ensuring efficient phase contact between rising vapour and descending liquid. The system is designed to produce a distillate with a high ethanol concentration while minimizing ethanol losses in the bottoms. The reflux ratio, theoretical and actual stage requirements, and column dimensions were determined using both hand calculations and ChemSep simulation, providing a comprehensive comparison of theoretical estimations and practical performance. This process is crucial in industries such as bioethanol production, pharmaceutical applications, and beverage distillation, where achieving high-purity ethanol is essential.

2. Distillation Column

2.1 Basis

Distillate flowrate, $D = 4\ kg/h$
Mole fraction of feed, $x_F=0.5$
Mole fraction of distillate, $x_D= 0.95$
Mole fraction of bottom, $x_B= 0.05$

Mass Balance

$F=D+B$
$F \cdot x_F=D \cdot x_D+B \cdot x_B$

Feed flowrate, *F*=8 *kg\/h*
Bottom flowrate, *B*=4 *kg\/h*

Vapour-Liquid Equilibrium Data

Temperature	x1	y1
K	mol fract.	
383.65	0	0
383.608	0.001	0.00232056
383.65	0	0
383.608	0.001	0.00232056
383.561	0.002	0.00463579
383.515	0.003	0.00694571
383.468	0.004	0.00925033
383.376	0.006	0.0138437
383.284	0.008	0.0184161
383.191	0.01	0.0229676
382.733	0.02	0.0454154
382.28	0.03	0.0673577
381.831	0.04	0.0888082
380.946	0.06	0.130287
380.079	0.08	0.169954
379.229	0.1	0.207905
377.175	0.15	0.295857
375.218	0.2	0.374907
373.351	0.25	0.44615
371.568	0.3	0.510525
369.865	0.35	0.568846
368.237	0.4	0.621814
366.677	0.45	0.670038
365.183	0.5	0.714046
363.749	0.55	0.754297
362.373	0.6	0.791193
361.051	0.65	0.825085
359.78	0.7	0.856282
358.556	0.75	0.885054
357.377	0.8	0.911639
356.241	0.85	0.93625
355.145	0.9	0.959073
354.717	0.92	0.967739
354.295	0.94	0.976156
353.879	0.96	0.984332
353.673	0.97	0.988333
353.468	0.98	0.992278
353.265	0.99	0.996166
353.225	0.992	0.996937
353.184	0.994	0.997706
353.144	0.996	0.998473

353.124	0.997	0.998856
353.103	0.998	0.999238
353.083	0.999	0.999619
353.058	1	1

Table 1: VLE Data

Relative Volatility, α

Relative volatility is a measure of how easily two components can be separated by distillation. It is defined as the ratio of the volatility (vapour pressures) of the more volatile component to the less volatile component.

$$\alpha = \frac{y/(1-y)}{x/(1-x)}$$

Where x and y are mole fractions of ethanol in liquid and vapour phase.
Relative volatility at feed, α_F
For x=0.5, corresponding y value from VLE data (table1) is 0.7
α=2.3

Reflux ratio, *R*

The reflux ratio is the ratio of liquid returned to the column to the liquid product withdrawn as distillate.

Minimum reflux ratio is found using the Underwood equation.

$$R_m = \sum \frac{\alpha_i \times x_{Di}}{\alpha_i - \theta} - 1$$

Where α_i is the relative volatility of component i
x_{Di} is the mole fraction of component i in distillate
θ is the Underwood root

To calculate the Underwood root, θ the below equation is used.

$$\sum \frac{\alpha_i \times x_{Fi}}{\alpha_i - \theta} = 1 - q$$

Where q is the feed quality factor. For a saturated feed q=1, for unsaturated feed q=0. In this problem 2/3 of the feed is in liquid state, therefore the value of q=0.67

θ=1.5

R_m=1.63

Actual reflux ratio is typically 1.2 – 2 times the minimum reflux ratio. A multiplying factor of 1.2 is assumed for determining the actual reflux ratio.

R=1.2×R_m
R=2

Theoretical Stages, *N*

A theoretical stage (or equilibrium stage) is where the vapour and liquid reach equilibrium.

To determine the minimum number of theoretical stages Fenske equation is used.

$$N_m = \frac{log\left[\left(\frac{x_D}{1-x_D}\right)\left(\frac{1-x_B}{x_B}\right)\right]}{log(\alpha)}$$

$$N_m = 7$$

To determine the actual number of theoretical stages Gilliland correlation is used.

$$\frac{N - N_m}{N+1} = 0.75 \times \left(\frac{R - R_m}{R+1}\right)^{0.5}$$

$$N = 9$$

Column Dimensions

Column height is calculated using the following formula.

H=(N×S)+$H_{allowances}$

Where S is stray spacing. A tray spacing of 0.7m is typically used for industrial scale distillation column, let $H_{allowances}$ (which accounts for Additional height for internals, feed zone, distributors, etc) be 2m.

H=8m

Column diameter is calculated using the following formula.

$$D = \sqrt{\frac{4A}{\pi}}$$

Where $A = \frac{V}{V_t}$
A is the area
V is the volumetric vapour flowrate
V_t is the maximum vapour velocity

Prerequisite parameters to determine column diameter include:
Molar flowrate of distillate, n_D

$$\dot{n}_D = \frac{D}{MW_i} + \frac{D}{MW_j}$$

D=4 *kg\/h*
MW_i=78 *kg/kmol*
MW_j=92 *kg/kmol*

n_D=0.09 *kmol/h*

Volumetric vapour flowrate, V

$$V = \frac{\dot{n}_D RT}{P}$$

$\dot{n}_D$=0.09 *kmol/h*
Universal gas constant, $R = 8.314\ m^3.kPa/kmol.K$
Operating temperature, $T = 93\ oC$ *or* $366\ K$
Operating pressure, $P = 1\ atm$ *or* $101.325\ kPa$

V=2.7 m^3/h

Maximum vapour velocity, V_t

$$V_t = C_S \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$$

Capacity factor, $C_S = 0.15\ (m/s)\ (m^3/kg)0.5$ *(for sieve trays)*
Density of liquid, $\rho_L = 798.8\ kg/m^3$
Density of vapour, $\rho_V = 2.8\ kg/m^3$

V_t=2.5 *m/s*=9000 *m/h*

Area, A

$$A = \frac{V}{V_t}$$
$$A = 0.003\ m^2$$

Substitute the Values to the Below Equation

$$D = \sqrt{\frac{4A}{\pi}}$$
$$D = 0.06\ m$$

Chem Sep Simulation

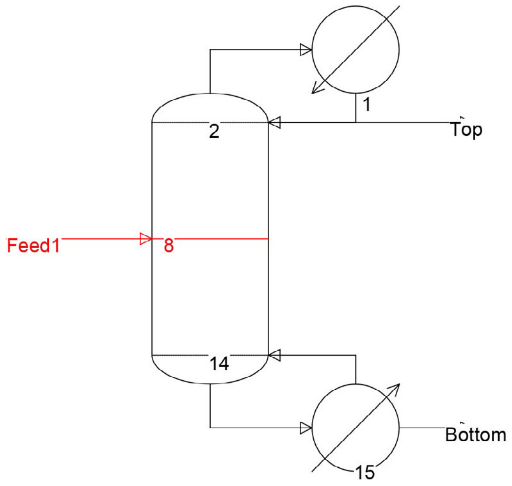


Figure 1: Operation Flowsheet

Column Configuration
Operation: Simple Distillation
Condenser: Total (Liquid product)
Reboiler: Partial (Liquid product)
Number of stages: 15
Feed stage(s): 8

Feed Stream(s) Specification
Stage: 8
Two-phase feed: Not-split
State: p and V
Pressure: 101.325 kPa
Vapour fraction (-): 0.33
Flowrate: 8.64189 kg/h

Thermodynamic Model
K-value: Wilson
Enthalpy: Excess

Column Specification
This distillation column operates at a constant, atmospheric pressure of 101.325 kPa, with no heat loss to the surroundings, and assumes perfect stage efficiency. A feed mixture is separated by vapour-liquid contact within the column, where more volatile components rise and condense at the top, while less volatile components descend. The condensed vapour is partially returned as reflux, and the remaining portion is withdrawn as distillate, while the bottom liquid is withdrawn as bottoms product, all under the maintained constant pressure.

Configuration

Operation: Simple Distillation

Condenser: Total (Liquid product)

Reboiler: Partial (Liquid product)

Number of stages (e.g. 10) 15

Feed stage(s) (e.g. 5,7) 8

Sidestream stage(s) (e.g. 2,9)

Pumparound(s) (e.g. 6>8, 9>1)

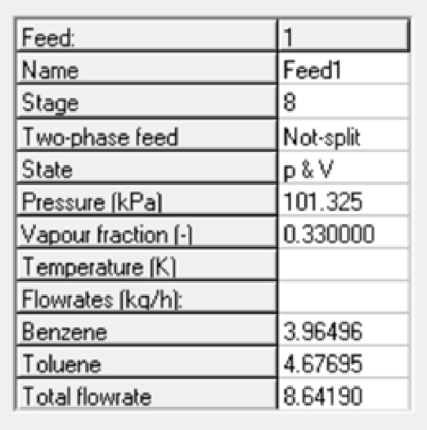
Interconnections

Extra condensers

Extra reboilers

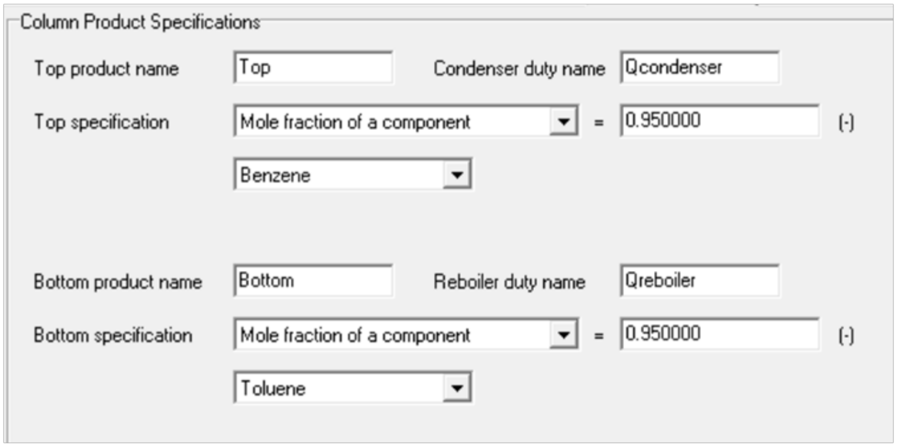
Drawing

Figure 2 : Column Configuration



Feed:	1
Name	Feed1
Stage	8
Two-phase feed	Not-split
State	p & V
Pressure (kPa)	101.325
Vapour fraction (-)	0.330000
Temperature (K)	
Flowrates (kg/h):	
Benzene	3.96496
Toluene	4.67695
Total flowrate	8.64190

Figure 3: Feed Stream Specification



Column Product Specifications

Top product name: Top

Condenser duty name: Qcondenser

Top specification: Mole fraction of a component = 0.950000 (-)

Benzene

Bottom product name: Bottom

Reboiler duty name: Qreboiler

Bottom specification: Mole fraction of a component = 0.950000 (-)

Toluene

Figure 4: Column Specifications

Stream	**Feed**	**V.Feed**	**L.Feed**	**Top**	**Bottom**
Stage	8	8	8	1	15
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325
Vapour fractioin (-)	0.33	1	0	0	0
Temperature (K)	366.302	366.302	366.302	352.923	380.562
Enthalpy (J/kmol)	-1.456 x 10^7	-	-	-2.593 x 10^7	-2.345 x 10^7

Total molar flow (kmol/s)	2.8200 x 10^-5	9.3060 x 10^-6	1.8894 x 10^-5	1.4100 x 10^-5	1.4100 x 10^-5
Total mass flow (kg/h)	8.64189	2.78379	5.85811	4.00056	4.64133
Vapour std.vol.flow (m^3/s)	2.2585 x 10^-4	2.2046 x 10^-4	-	-	-
Liquid std.vol.flow (m^3/s)	1.8393 x 10^-6	-	1.8609 x 10^-6	1.2607 x 10^-6	1.4817 x 10^-6
Vapour:					
Mole weight (kg/kmol)	83.0942	83.0942	-	-	-
Density (kg/m^3)	2.85114	2.85114	-	-	-
Std.density (kg/m^3)	3.50749	3.50749	-	-	-
Viscosity (N/m^2.s)	9.0202 x 10^-6	9.0202 x 10^-6	-	-	-
Heat capacity (J/kmol/K)	112434	112434	-	-	-
Thermal cond. (J/s/m/K)	0.0174483	0.0174483	-	-	-
Liquid:					
Mole weight (kg/kmol)	86.1255	-	86.1255	78.8132	91.4371
Density (kg/m^3)	798.837	-	798.837	812.967	783.917
Std.density (kg/m^3)	874.427	-	874.427	881.407	870.112
Viscosity (N/m^2.s)	2.7997 x 10^-4	-	2.7997 x 10^-4	3.1786 x 10^-4	2.4367 x 10^-4
Heat capacity (J/kmol/K)	166938	-	166938	150580	181420
Thermal cond. (J/s/m/K)	0.116339	-	0.116339	0.123519	0.110596
Surface tension (N/m)	0.0197980	-	0.0197980	0.0211918	0.0184278

Table 2: Streams

McCabe-Thiele Plot

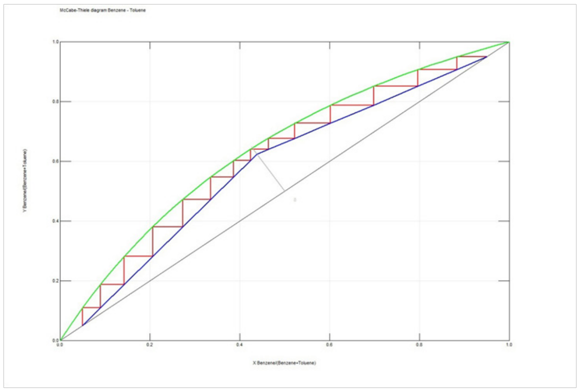


Figure 5: McCabe-Thiele Diagram Benzene-Toluene

Binary Phase Diagram

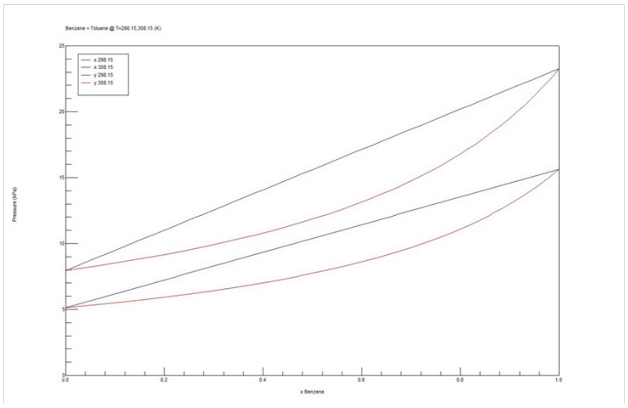
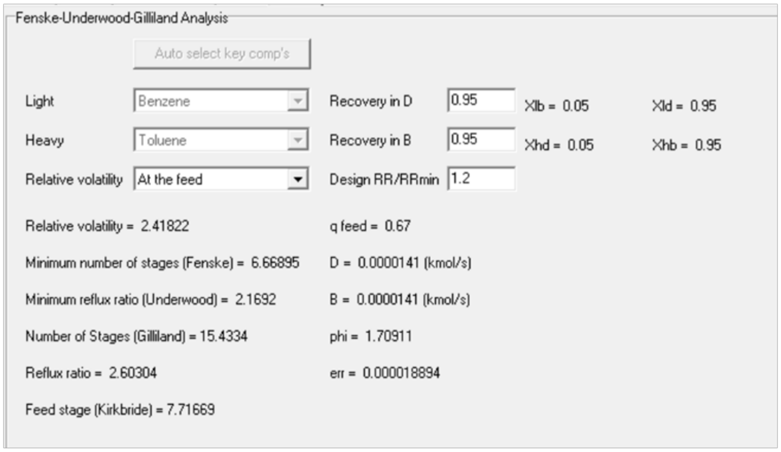


Figure 6: Phase Diagram Benzene-Toluene

Fenske-Underwood-Gilliland Analysis



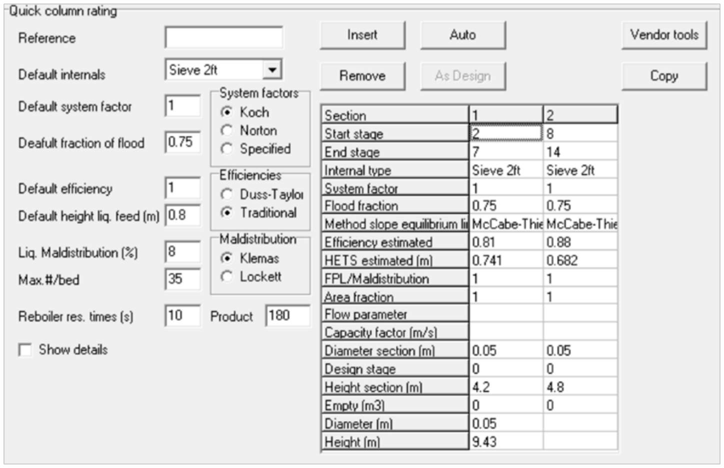
Fenske-Underwood-Gilliland Analysis

Light: Benzene
Heavy: Toluene
Relative volatility: At the feed
Recovery in D: 0.95
Recovery in B: 0.95
Design RR/RRmin: 1.2
Xlb = 0.05
Xhd = 0.05
Xld = 0.95
Xhb = 0.95

Relative volatility = 2.41822
Minimum number of stages (Fenske) = 6.66895
Minimum reflux ratio (Underwood) = 2.1692
Number of Stages (Gilliland) = 15.4334
Reflux ratio = 2.60304
Feed stage (Kirkbride) = 7.71669
q feed = 0.67
D = 0.0000141 (kmol/s)
B = 0.0000141 (kmol/s)
phi = 1.70911
err = 0.000018894

Figure 7: Fenske-Underwood-Gilliland Analysis

Column Dimensions



Quick column rating

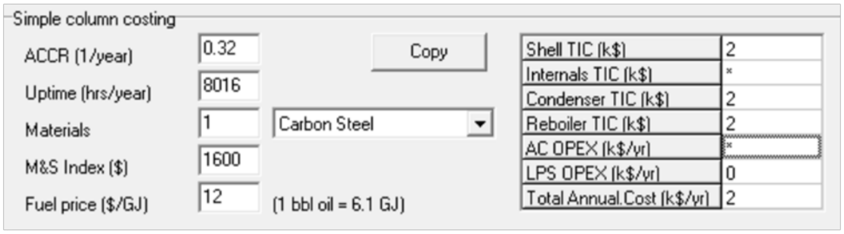
Reference:
Default internals: Sieve 2ft
Default system factor: 1
Deafult fraction of flood: 0.75
Default efficiency: 1
Default height liq. feed (m): 0.8
Liq. Maldistribution (%): 8
Max.#/bed: 35
Reboiler res. times (s): 10
Product: 180
☐ Show details

System factors: ● Koch ○ Norton ○ Specified
Efficiencies: ○ Duss-Taylor ● Traditional
Maldistribution: ● Klemas ○ Lockett

Section	1	2
Start stage	2	8
End stage	7	14
Internal type	Sieve 2ft	Sieve 2ft
System factor	1	1
Flood fraction	0.75	0.75
Method slope equilibrium li	McCabe-Thie	McCabe-Thie
Efficiency estimated	0.81	0.88
HETS estimated (m)	0.741	0.682
FPL/Maldistribution	1	1
Area fraction	1	1
Flow parameter		
Capacity factor (m/s)		
Diameter section (m)	0.05	0.05
Design stage	0	0
Height section (m)	4.2	4.8
Empty (m3)	0	0
Diameter (m)	0.05	
Height (m)	9.43	

Figure 8: Column Dimensions

Cost of Construction



Simple column costing

ACCR (1/year): 0.32
Uptime (hrs/year): 8016
Materials: 1 Carbon Steel
M&S Index ($): 1600
Fuel price ($/GJ): 12 (1 bbl oil = 6.1 GJ)

Shell TIC (k$)	2
Internals TIC (k$)	*
Condenser TIC (k$)	2
Reboiler TIC (k$)	2
AC OPEX (k$/yr)	*
LPS OPEX (k$/yr)	0
Total Annual Cost (k$/yr)	2

Figure 9: Cost of Construction

3. Summary

The rough calculations and the ChemSep simulation provide different levels of detail and accuracy in the distillation column design. The rough calculations use fundamental mass balances and relative volatility assumptions to determine key parameters such as reflux ratio (R = 2), theoretical stages (7), and actual trays (10). In contrast, the simulation accounts for detailed vapour-liquid equilibrium (VLE) using the Wilson model, leading to a slightly different number of trays (15) and a more refined feed stage placement (stage 8). While the rough method assumes a constant relative volatility ($\alpha = 2.3$), the simulation dynamically calculates phase equilibrium, leading to potential deviations in separation performance. Additionally, column dimensions differ slightly, with the rough calculation estimating a height of 8 m and a diameter of 0.06 m, whereas the simulation provides detailed vapour flow and liquid density data but does not explicitly state the diameter. The energy balance is also more comprehensive in the simulation, incorporating enthalpy and heat capacity values rather than simple approximations. These differences highlight the importance of simulation in refining design parameters beyond initial hand calculations.

The key differences between the rough calculations and the ChemSep simulation lie in accuracy, design parameters, and energy considerations. The rough calculations assume a constant relative volatility ($\alpha = 2.3$) and use simplified VLE data, whereas the simulation employs the Wilson model for a more precise phase equilibrium representation. In terms of reflux ratio and tray count, the rough approach estimates a minimum reflux ratio ($R_m = 1.63$) and selects an actual reflux ratio of 2, leading to 9 theoretical stages and 10 trays, while the simulation, using iterative calculations, results in a 15-tray column with the feed at stage 8. Column dimensions also differ, with the rough calculation estimating a height of 8 m and a diameter of 0.06 m, while the simulation provides detailed vapour flow and density data but does not explicitly state the diameter. Energy balance considerations further highlight the difference, as the rough method does not explicitly calculate energy requirements, whereas the simulation accounts for enthalpy, heat capacities, and temperature variations, offering a more realistic energy balance. Finally, the simulation enhances separation feasibility analysis by providing a McCabe-Thiele plot, phase diagrams, and detailed component balances, whereas the rough calculation relies on the Fenske-Underwood-Gilliland method for estimating theoretical and actual stages. The simulation results indicate a slightly higher number of trays (15 vs. 10 from hand calculations) due to more accurate VLE modeling. The reflux ratio and energy balance considerations also show minor deviations, highlighting the importance of detailed thermodynamic modeling.

3.1 Industrial Relevance & Practical Considerations

The ethanol-water distillation process is widely used in industries such as bioethanol production, pharmaceutical manufacturing, and beverage distillation. Achieving high-purity ethanol (96% or higher) is essential for fuel blending, medical-grade alcohol, and alcoholic beverages. In industrial settings, distillation columns must be optimized for energy efficiency, as reboiler and condenser duties significantly impact operating costs. Additionally, tray efficiency, column pressure, and material selection are crucial for long-term performance and corrosion resistance. Stainless steel (SS 304 or SS 316) is commonly used for ethanol distillation due to its corrosion resistance, durability, and compliance with food-grade standards. Other factors such as scalability, automation, and waste management must be considered to ensure cost-effective and sustainable operation.

3.2 Estimated Cost of Construction (in INR)

The cost of constructing a distillation column depends on materials, fabrication, installation, and auxiliary components such as reboilers, condensers, and instrumentation. Below is a rough cost estimate based on common industrial practices [1-10].

3.2.1. Column Shell & Trays

- Material: Stainless Steel (SS 304)
- Height: 9.5 m, Diameter: 0.05 m
- Plate Type: Sieve trays (10 trays)

Component	**Specification**	**Approximate Cost (INR)**
SS 304 Shell & Fabrication	9.5m height, 0.05m dia	₹3,90,000
Trays (Sieve Type)	10 trays	₹1,00,000
Support Structures & Insulation	Mild Steel + Coating	₹50,000

3.2.2 Reboiler & Condenser

- Reboiler Type: Kettle-type
- Condenser Type: Total condenser

Component	**Specification**	**Approximate Cost (INR)**
Reboiler (Kettle-Type, SS 304)	100 L capacity	₹1,80,000
Condenser (Shell & Tube, SS 304)	Heat duty ~5 kW	₹1,50,000

3.2.3. Pumps, Piping & Instrumentation

- Valves, flow meters, temperature & pressure sensors

Component	**Specification**	**Approximate Cost (INR)**
Pumps (Feed & Reflux)	SS 304, 1-2 HP	₹70,000
Piping & Valves	SS 304, ~50m length	₹1,20,000
Instrumentation (Sensors, Controllers)	Temperature, Pressure, Flow meters	₹1,00,000

3.2.4. Installation & Miscellaneous Costs

Category	**Approximate Cost (INR)**
Fabrication & Installation	₹2,00,000
Automation & Control Systems	₹1,50,000
Safety Equipment & Miscellaneous	₹50,000

Total Estimated Cost

₹11,38,000 (11.38 Lakhs INR)

(The cost may vary based on fabrication charges, raw material price fluctuations, and specific process requirements.)

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