# CHE453: Capstone Project

# Bi-weekly report number: 1

***Team members:***

| | |
|---|---|
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***Project title:***

Production of Methyl Benzoate via Esterification of Benzoic Acid with Methanol

***Objectives for this report:***

1. **Process Identification:** Esterification to produce Methyl Benzoate
2. **Specifications of Product and Feed Streams:**
    a. Feed Streams: Methanol (16.95k moles), Benzoic Acid (with 0.5 mass% impurity of Phthalic Acid) (2.7k moles)
    b. Product Stream: Methyl Benzoate (7352.94 + 0.0029k moles) (Some Benzoic Acid Leakage)

    Note: k is a scaling factor to be determined by simulations

3. **Block Diagram**

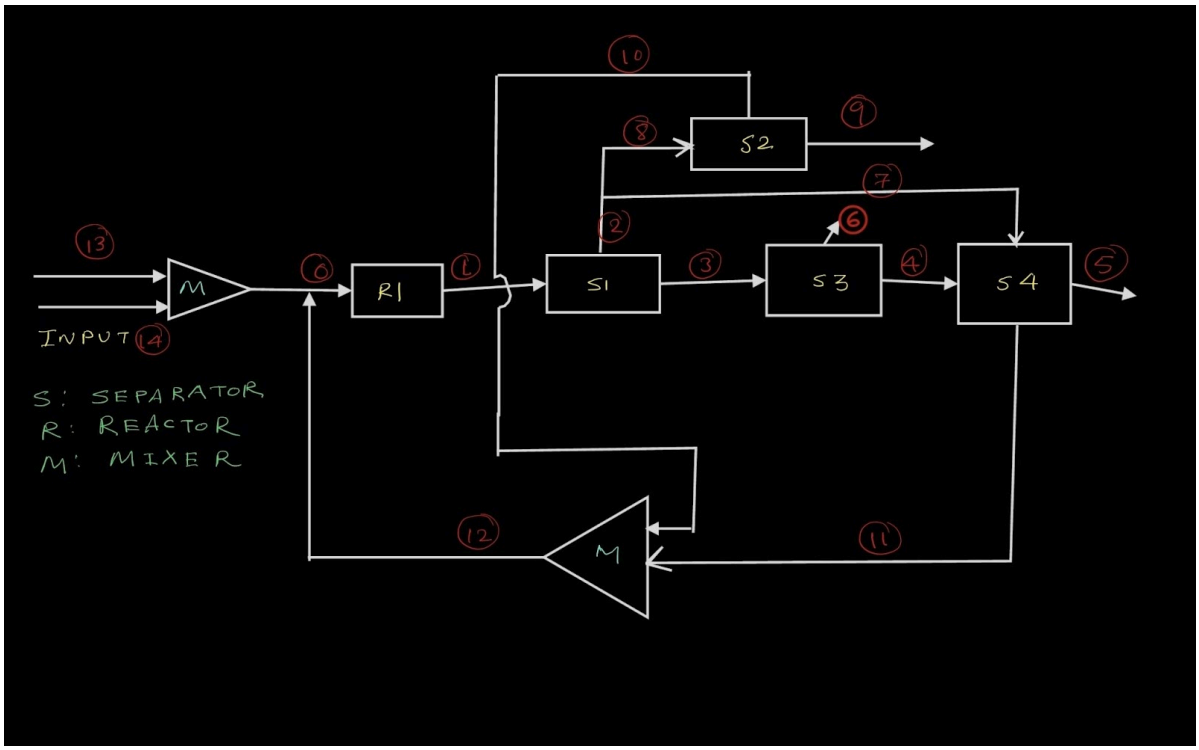



**Figure 1**

| | Input | 0 | 1 | 2 | 3 |
|---|---|---|---|---|---|
| Methanol | 16.95k | 52057.16 | 44621.603 | 44621.603 | 0 |
| Benzoic Acid | 2.69k | 8261.73 | 826.173 | 0 | 826.173 |
| Phthalic Acid | 0.01k | 0.01k | 0.01k | 0 | 0.01k |
| Methyl Benzoate | 0 | 0 | 7435.557 | 0 | 7435.557 |
| Water | 0 | 0 | 7435.557 | 7435.557 | 0 |

| | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|
| Methanol | 0 | t(44621.603) | 0 | t(44621.603) | (1-t)(44621.603) |
| Benzoic Acid | 0.000345k + 822.042 | 0 | 4.131 - 0.000345k | 0 | 0 |
| Phthalic Acid | 0.01k | 0.01k | 0 | 0 | 0 |
| Methyl Benzoate | 74.356 - 0.00021k | 0 | 0.0029k + 7352.94 | 0 | 0 |
| Water | 0 | t(7435.557) | 0 | t(7435.557) | (1-t)(7435.557) |

| | 9 | 10 | 11 | 12 |
|---|---|---|---|---|
| Methanol | (1-t)(44621.603) - (52057.16 - 16.95k) | (52057.16 - 16.95k) | 0 | (52057.16 - 16.95k) |
| Benzoic Acid | 0 | 0 | (8261.73 - 2.69k) | (8261.73 - 2.69k) |
| Phthalic Acid | 0 | 0 | 0 | 0 |
| Methyl Benzoate | 0 | 0 | 0 | 0 |
| Water | (1-t)(7435.557) | 0 | 0 | 0 |

Note: k is a scaling factor to be determined by simulations, t is to be determined using Aspen Plus

## 4. Input-output cost analysis & preliminary economic feasibility:

a. Market Trends and Demand Analysis:

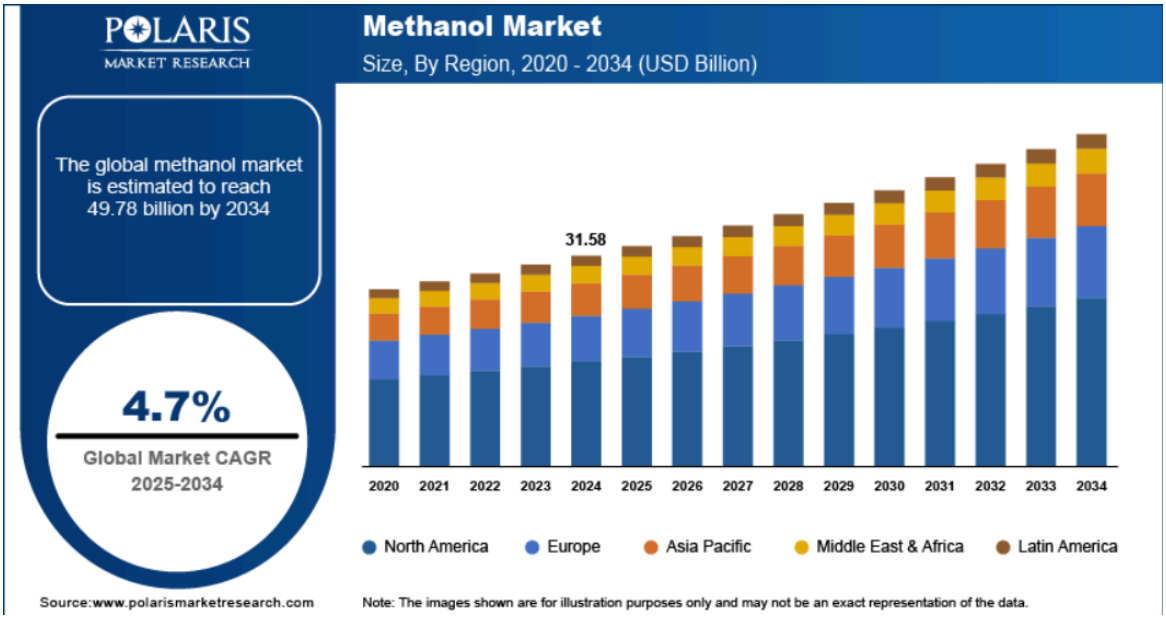
Methanol

- USD 370/MT — Asia Pacific (valid August 1–31, 2025), as posted by Methanex.
- USD 345/MT — Quarter-ending price for methanol CFR Nagoya, Japan (July 2025) ChemAnalyst.

Estimated Range: USD 345–370 per metric ton

**Market Trend ( Source: https://www.polarismarketresearch.com/industry-analysis/methanol-market )**

The global methanol market size was valued at USD 31.58 billion in 2024. The market is projected to grow from USD 33.01 billion in 2025 to USD 49.78 billion by 2034, exhibiting a CAGR of 4.7% during 2025–2034.




Methanol market drivers are as follows –

1. Rising Adoption of Methanol as Clean Fuel Alternative
2. Increasing Shift Toward Bio-Methanol and Green Methanol
3. Growing Applications in Production of Olefins and Aromatics as olefins are critical feedstocks for plastics, chemicals, and synthetic materials.

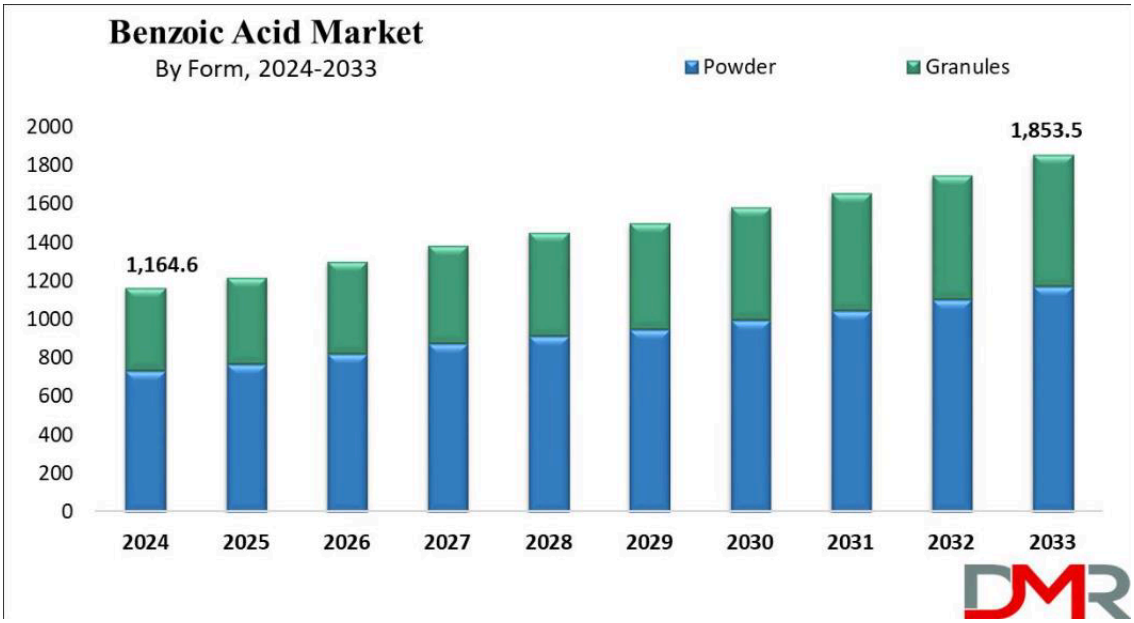
Benzoic Acid

- USD 1,010/MT — FOB Shanghai, average for Q1 2025 ChemAnalyst.
- USD 1,140/MT — China Q2 2024 IMARC Group.
- USD 2,252.54/MT — India Q4 2023 Credence Research Inc. (Note: as of late 2023; likely higher due to historical context).

Estimated Range (Recent): USD 1,010–1,140 per metric ton (current best estimate)

**Market Trend ( Source: https://dimensionmarketresearch.com/report/benzoic-acid-market )**

The Global Benzoic Acid Market size was valued at USD 1,104.4 million by the end of 2023 and is further anticipated to grow to a market value of USD 1853.5 million by 2033, at a CAGR of 5.3%.




Benzoic acid market drivers are as follows –

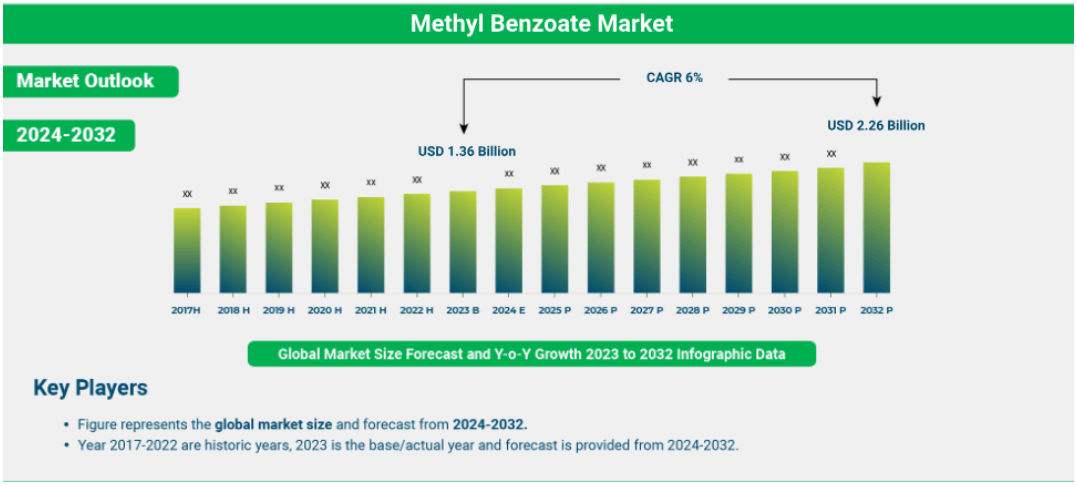
1. Use cases in production of ointments which are antifungal, & are applied to treat many skin conditions like fungal infections, insect bites, ringworms, & burns.
2. Application in food items for their strong antimicrobial properties.
3. Industrial applications such as production of benzoyl chloride, which is essential in the manufacture of dyes, perfumes, and other organic compounds.

## Methyl Benzoate

- USD 2,200/MT — Industrial-grade Methyl Benzoate in Q4 2023 Datavagyanik.

Estimated Price: Around USD 2,200 per metric ton (as no later APAC-specific data is available)

**Market Trend ( Source: https://dataintelo.com/report/global-methyl-benzoate-market )**The global methyl benzoate market size was USD 1360 million in 2023 and is likely to reach USD 2260 million by 2032, expanding at a CAGR of 6% during 2024–2032.




Methyl Benzoate market drivers are as follows –

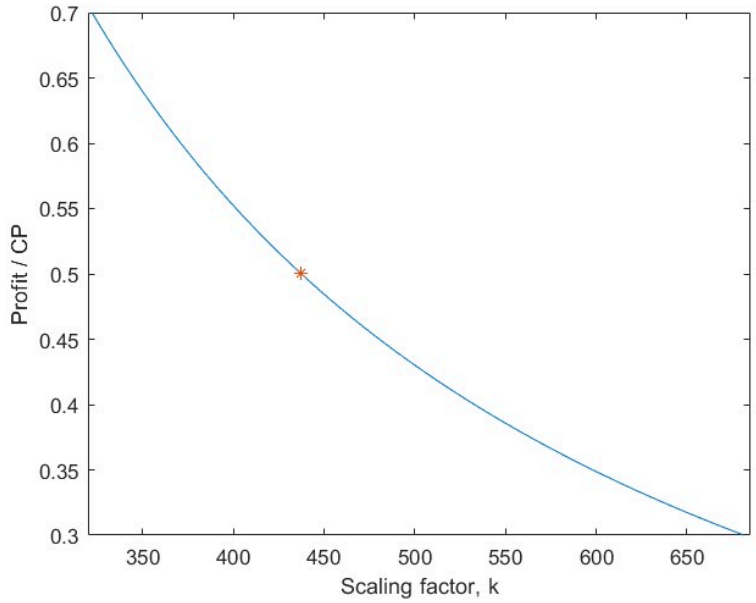
1. Increasing demand in the fragrance and flavor industry.
2. Growing applications as a solvent and intermediate in pharmaceuticals, agrochemicals, and other industries.
3. In the pharmaceutical sector, Methyl Benzoate serves as a key ingredient in various drug formulations, including topical analgesics and antiseptics, owing to its antifungal and antibacterial properties.

## b. Cost Tabulation and Demo optimisation:

| | Benzoic Acid | | Methanol | | Methyl Benzoate | | |
|---|---|---|---|---|---|---|---|
| | | | | | | | Molar Efficiency |
| MW(gm/mole) | 122.12 | | 32.04 | | 136.15 | | 0.9 |
| Mass(kg) | 996.61 | | 1641.02 | | | | |
| Raw Mass(kg) | 1001.62 | | 1641.02 | | 1000.00 | | |
| Mole | 8160.91 | | 51217.79 | | 7344.82 | | Methanol Purity |
| Excess Mole | 0.00 | | 43056.88 | | | | 1 |
| Raw Mass(MTon) | 1.00161809 | | 1.641018026 | | 1.00 | | |
| Cost(USD/MT) | 1010.00 | | 370.00 | | 2200.00 | | Benzoic Acid Purity |
| UnReacted Mole | 816.09 | | 43872.97 | | | | 0.995 |
| UnReacted Mass(Mton) | 0.10 | | 1.41 | | | | |
| Total Cost(USD) | 1011.634271 | | 607.1766696 | | 2199.99 | | |
| | | | | | | | MeOH:BnZ_A |
| | | | | | | | 1.6466 |
| Total Input Cost(USD) | 1618.81 | | | | | | |
| Excess Reactant Cost(USD) | 620.76 | | | | | | |
| Total Output Cost(USD) | 2199.99 | | | | | | |
| Net Profit | 2820.76 | | | | | | |
| Profit (x) | 1.742486281 | | | | | | |

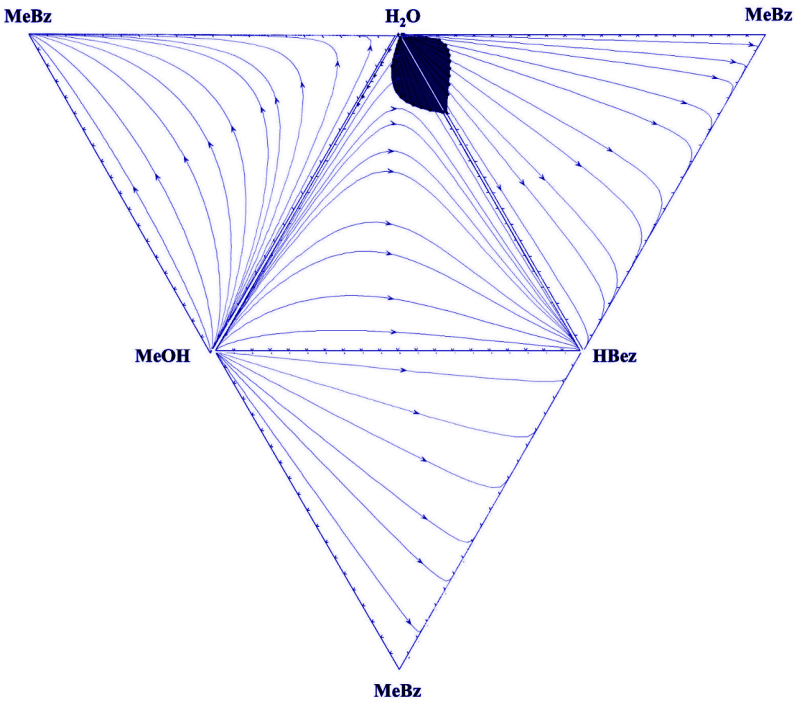
c. Selection of k using profitability:

| | | | | |
|---|---|---|---|---|
| Benzoic Acid | 2.7k | 1.01 | 0.122 | 0.33k |
| Methanol | 16.95k | 0.37 | 0.032 | 0.2k |
| Methyl Benzoate | 0.0029k + 7352.94 | 2.2 | 0.136 | 0.0009k + 2200 |
| | | Profit | 2200 - 0.529k | |

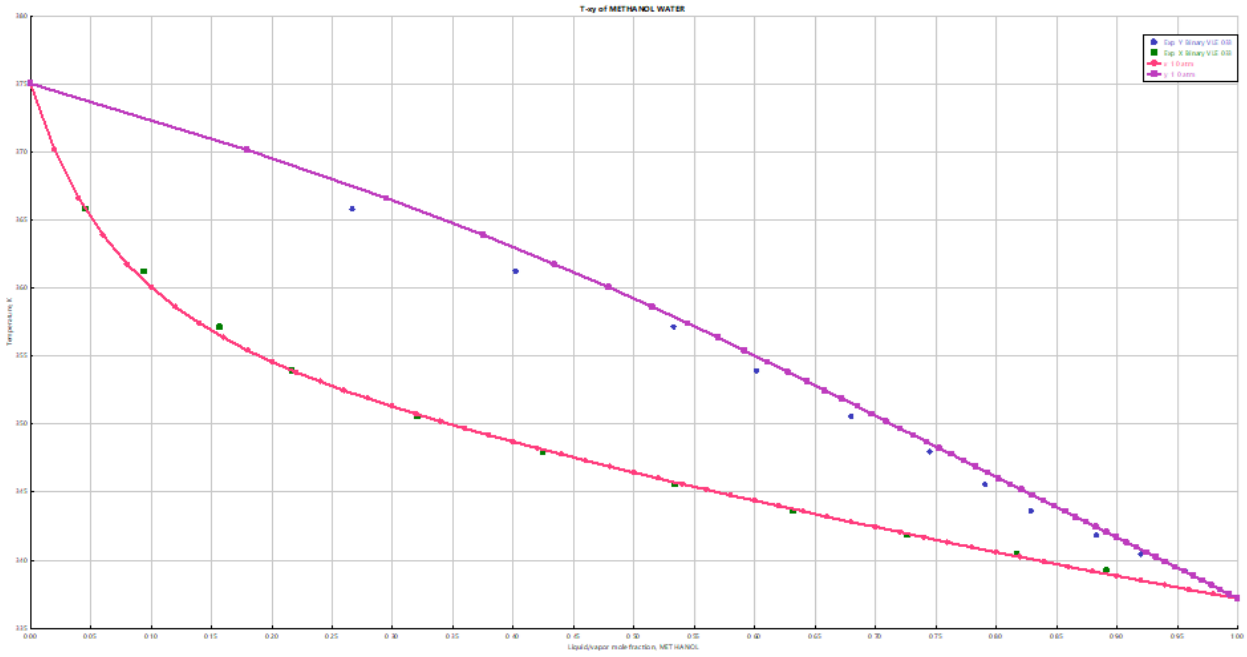



Break Even Point: at Profit:CP = 0.5, k = 437

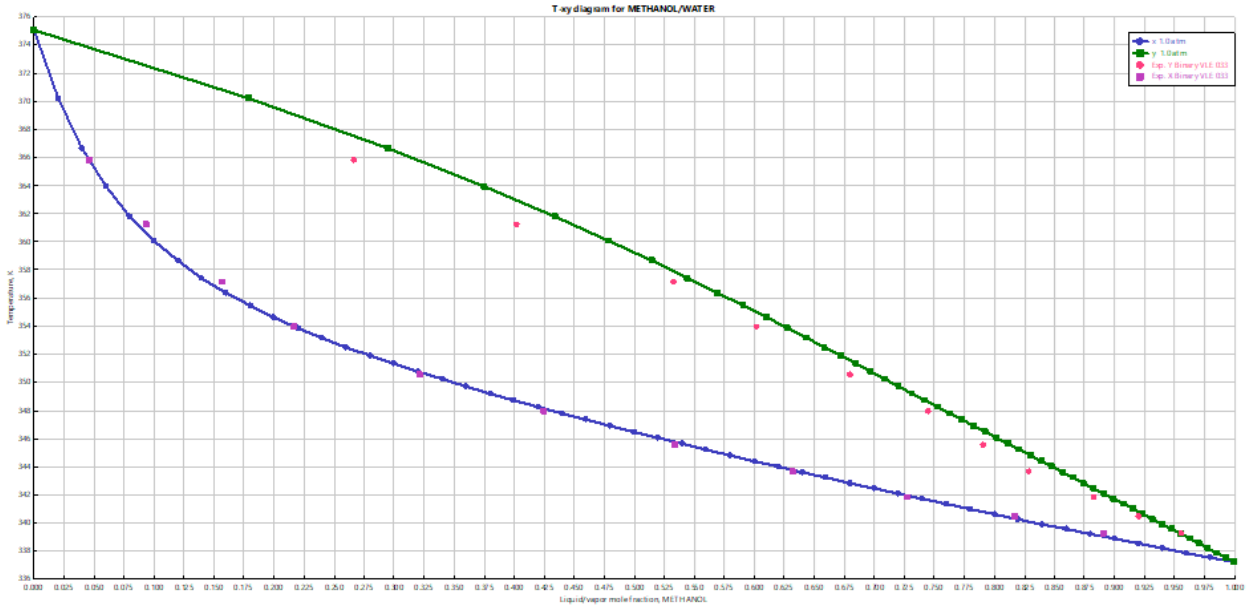
## 5. Thermodynamic model selection and validation



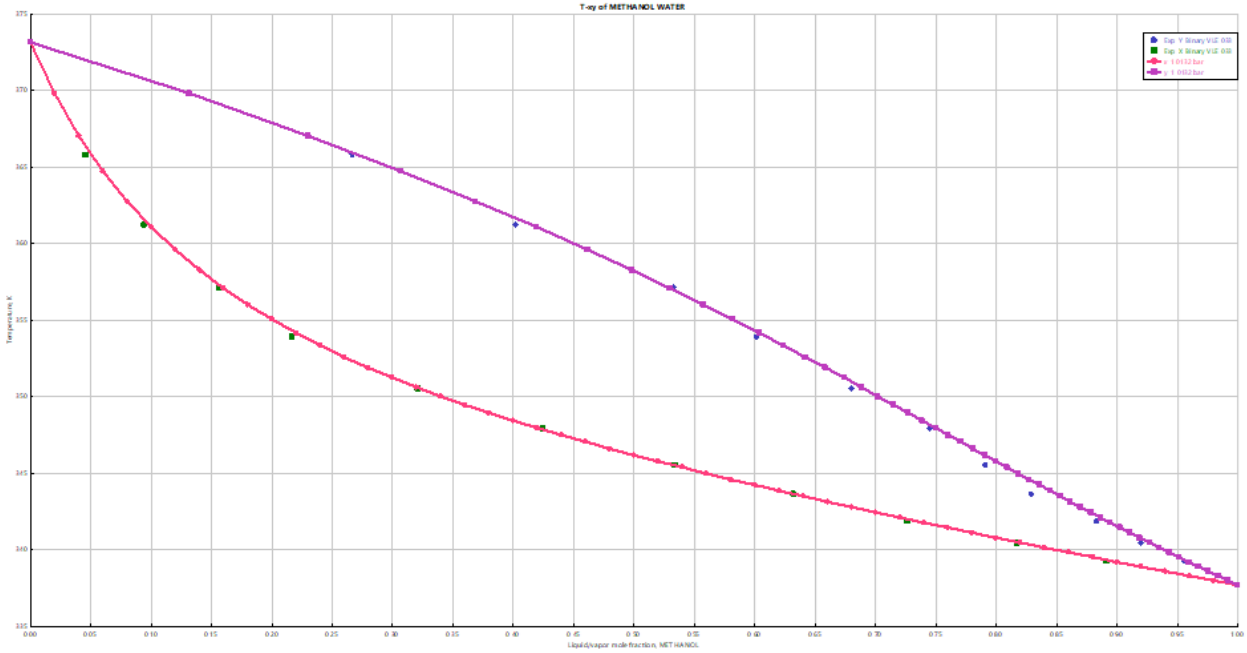

## Thermodynamic Methods (Water - Methanol Binary Mixture)




## NRTL



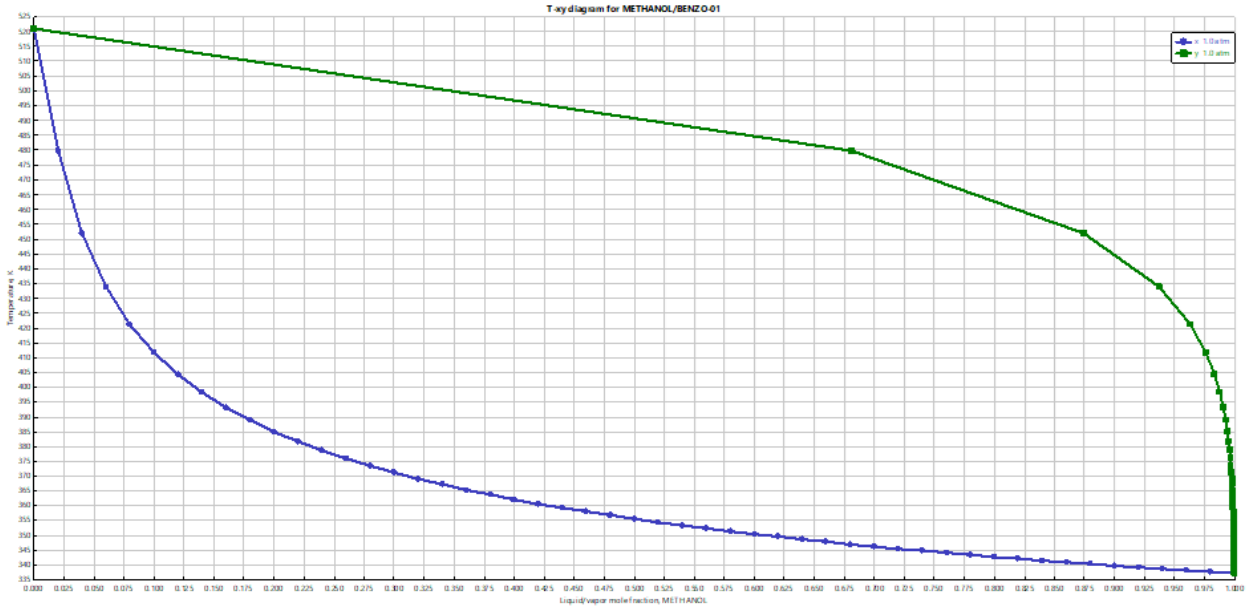

**PENG-ROB**



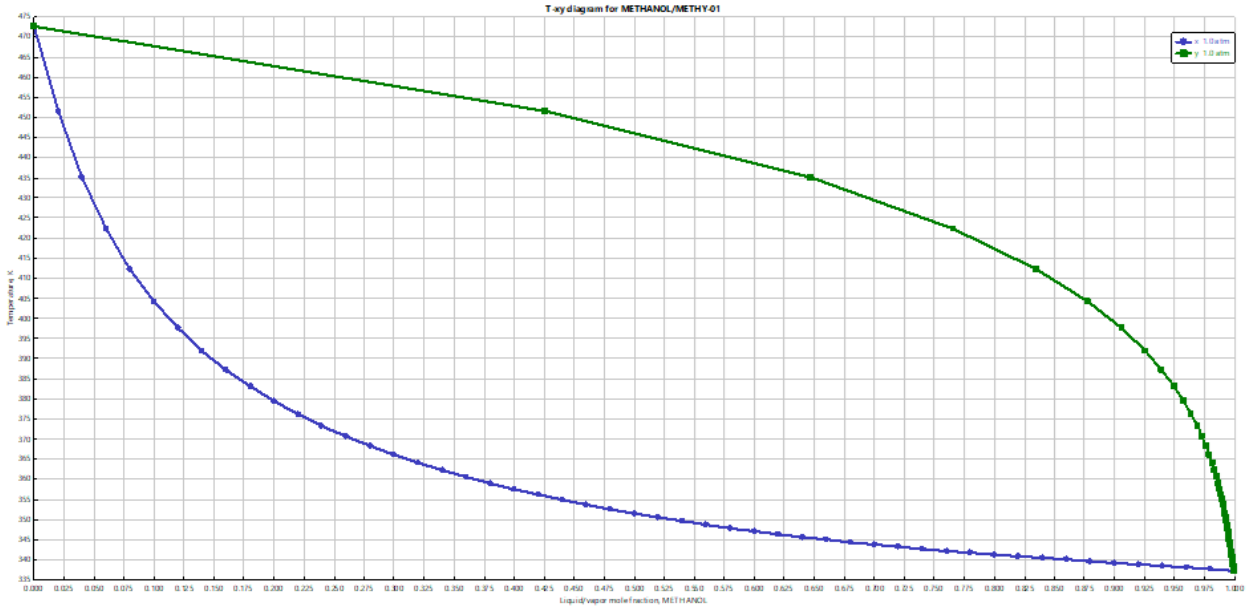

**UNIQUAC**

**** From the above thermodynamic methods, UNIQUAC method is the best as it fits the above test.***

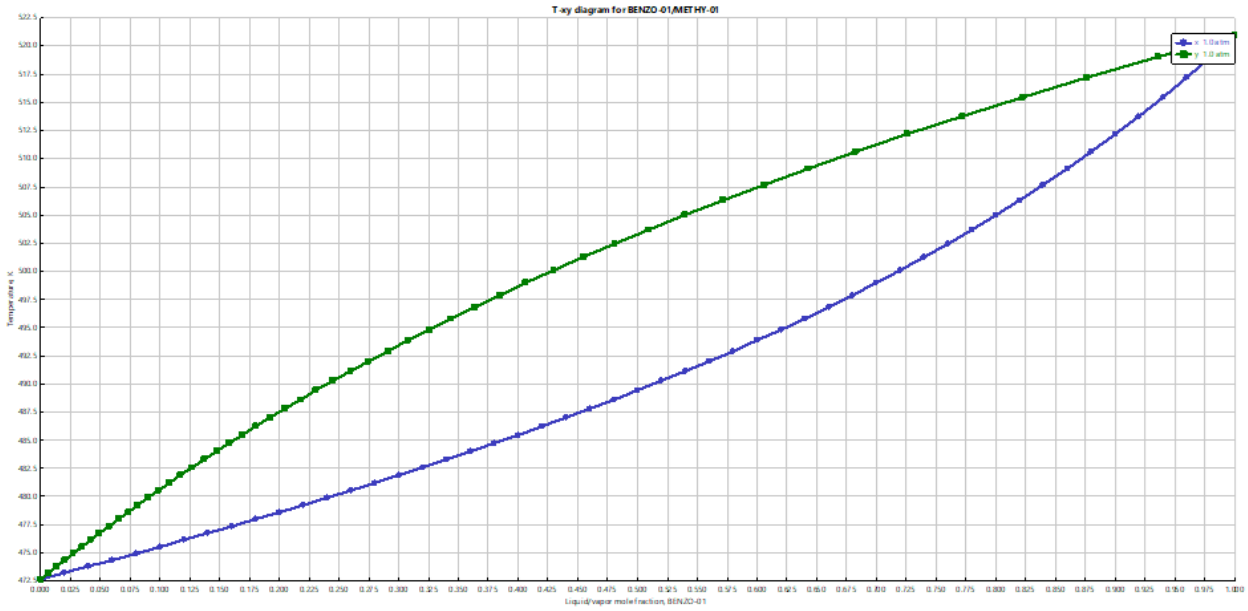
# Txy Plots



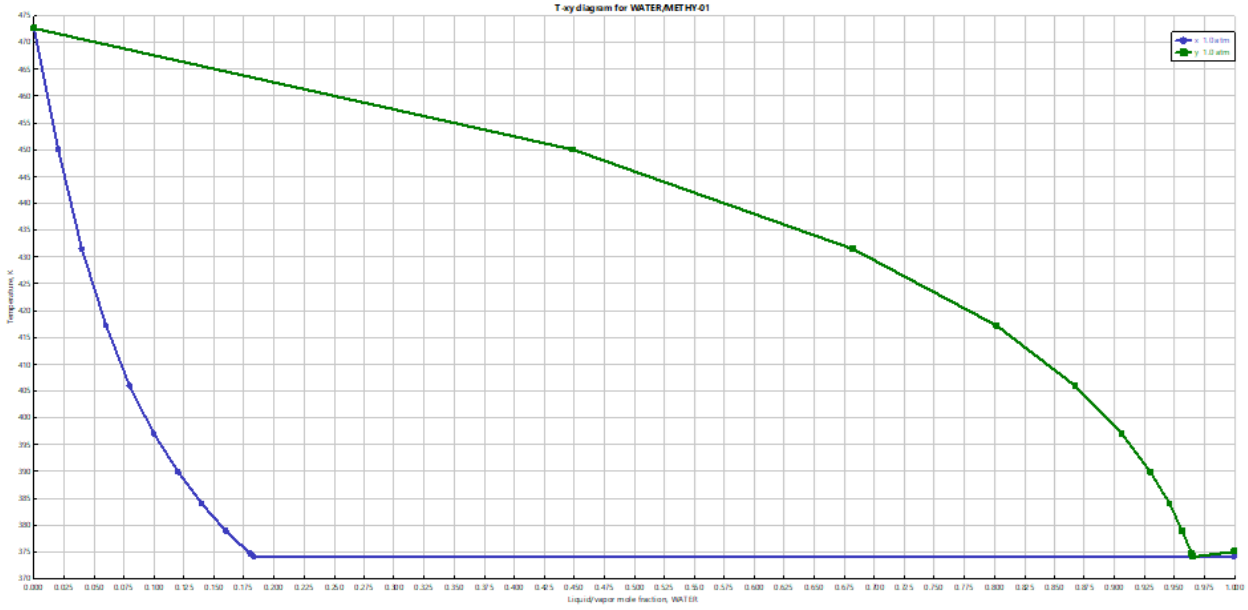

**Txy (Methanol and Benzoic Acid)**



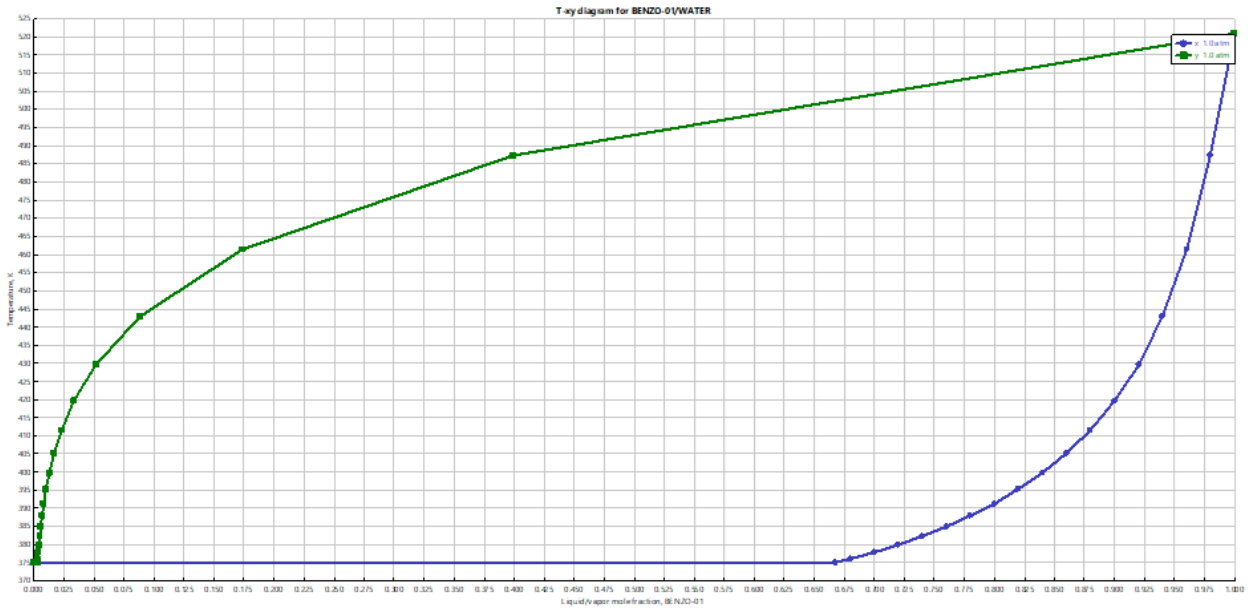

**Txy (Methanol and Methyl Benzoate)**




**Txy (Benzoic Acid and Methyl Benzoate)**




**Txy (Water and Methyl Benzoate)**




**Txy (Benzoic Acid and Water)**

## AZEOTROPE IDENTIFICATION

**AZEOTROPE SEARCH REPORT**

**Physical Property Model:** UNIQUAC **Valid Phase:** VAP-LIQ

***Mixture Investigated For Azeotropes At A Pressure Of 101325 N/SQM***

| Comp ID | Component Name | Classification | Temperature |
|---|---|---|---|
| METHANOL | METHANOL | Unstable node | 64.53 C |
| WATER | WATER | Saddle | 100.02 C |
| BENZO-01 | BENZOIC-ACID | Stable node | 248.93 C |
| METHY-01 | METHYL-BENZOATE | Saddle | 199.31 C |

***No Azeotropes Were Found***

**AZEOTROPE SEARCH REPORT**

**Physical Property Model:** UNIQUAC **Valid Phase:** VAP-LIQ

***Mixture Investigated For Azeotropes At A Pressure Of 5 BAR***

| Comp ID | Component Name | Classification | Temperature |
|---|---|---|---|
| METHANOL | METHANOL | Unstable node | 111.52 C |
| WATER | WATER | Saddle | 151.92 C |
| BENZO-01 | BENZOIC-ACID | Stable node | 319.17 C |
| METHY-01 | METHYL-BENZOATE | Saddle | 278.74 C |

***No Azeotropes Were Found***

**AZEOTROPE SEARCH REPORT**

**Physical Property Model:** UNIQUAC **Valid Phase:** VAP-LIQ

***Mixture Investigated For Azeotropes At A Pressure Of 10 BAR***

| Comp ID | Component Name | Classification | Temperature |
|---|---|---|---|
| METHANOL | METHANOL | Unstable node | 136.81 C |
| WATER | WATER | Saddle | 179.98 C |
| BENZO-01 | BENZOIC-ACID | Stable node | 358.70 C |
| METHY-01 | METHYL-BENZOATE | Saddle | 323.44 C |

***No Azeotropes Were Found***

Results with short discussion:

In this bi-weekly report, we successfully identified the esterification process for producing Methyl Benzoate from Benzoic Acid and Methanol, with detailed specifications for feed streams (Methanol: 16.95k moles, Benzoic Acid: 2.7k moles with 0.5 mass% Phthalic Acid impurity) and product stream (Methyl Benzoate: 7352.94 + 0.0029k moles, with minor Benzoic Acid leakage). The block diagram was developed, illustrating stream compositions across units (e.g., reactor R1 converting feeds to 7435.557 moles each of Methyl Benzoate and Water), and a scaling factor k was introduced for simulation-based optimization. Economic analysis revealed strong market growth for all components—Methanol projected to reach USD 49.78 billion by 2034 at 4.7% CAGR, Benzoic Acid to USD 1,853.5 million by 2033 at 5.3% CAGR, and Methyl Benzoate to USD 2,260 million by 2032 at 6% CAGR—with input costs at USD 198.47 (including excess reactant USD 76.07), output at USD 1,980.00, yielding a net profit of USD 2,056.07 and a profit multiplier of 10.36. Break-even analysis determined k ≈ 1,199 for a Profit:CP ratio of 0.5. Thermodynamic modeling validated UNIQUAC as the optimal method over NRTL and PENG-ROB based on fitting tests, supported by Txy plots for key binary mixtures (Water-Methanol). Azeotrope searches confirmed no azeotropes in investigated mixtures under UNIQUAC, VAP-LIQ, and VAP-UQ phases, simplifying separation processes.

Objectives which could not be accomplished with reasons:

- Scaling Factor has to be calculated using aspen simulation and block-wise optimisation.
- Exact real time cost calculation could be done, only after determining k and t.
- Cross validation of cost could not be done with real data due to some conflicts that have to be removed.

Any other challenges:

- Unavailability of Experimental Data for Benzoic Acid or Methyl Benzoate based binary mixtures, hindering validation during Thermodynamic Analysis.
- Lack of recent Literature and Industrial data of Fischer Esterification using these data

Bibliography:

A Study of the Esterification of Benzoic Acid with Methyl Alcohol Using Isotopic Oxygen, Irving Roberts and Harold C. Urey

Continuous Process for Preparing, Wesley Wayne McConnell and Bruce Edward Stanhope (Grayslake, IL), Josef L. Luxem (Palatine, IL)

Number of hours spent on Capstone project during this period: 26 hours total

Contributions from individual members:

1. Aaditya Amlan Panda (Block Diagram Visualisation)
2. Abhijit Dalai (Flowsheeting Optimisation)
3. Adarsh Pal  (Block Diagram Visualisation)
4. Akash Kumar Gupta (Flowsheeting Optimisation)
5. Kushagra Tiwari (Thermodynamic Analysis)
6. Saurabh Yadav (Market and Profitability Analysis)
7. Snehil Tripathi (Market and Profitability Analysis)
8. Tushar Verma (Thermodynamic Analysis)

Signatures of members:

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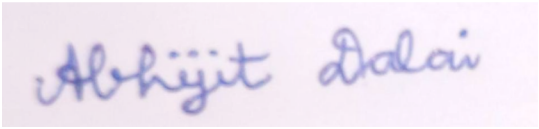
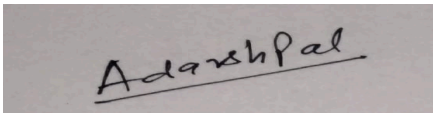
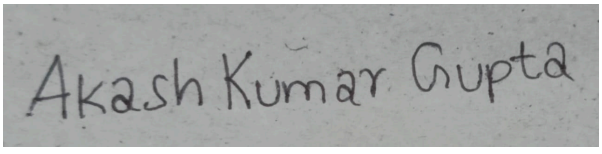
|---|---|
| Aaditya Amlan Panda |  |
| Abhijit Dalai |  |
| Adarsh Pal |  |
| Akash Kumar Gupta |  |

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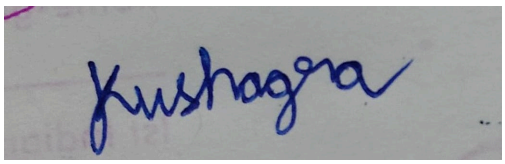
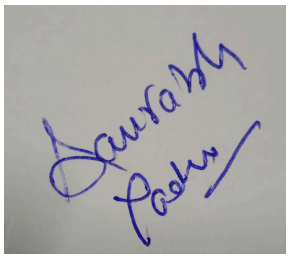
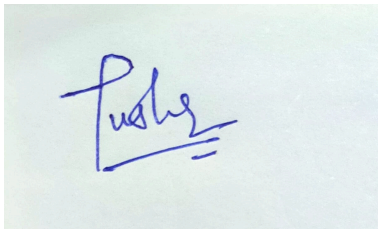
| Kushagra Tiwari |  |
| Saurabh Yadav |  |
| Snehil Tripathi |  |
| Tushar Verma |  |