Optimization in Application: Green Epichlorohydrin Plant Production

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AGENDA

1. Problem & Motivation
2. Data for Problem
3. Method to Solve
4. Key Findings
5. Conclusion

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Problem & Motivation

Network representation of chemical plant

5 total materials
2 reactants
1 final product

ECH is a primary intermediate in epoxy resin production

- ECH traditionally produced using propylene
- Glycerol sustainable alternative (biodiesel byproduct)

Plant centered around dehydrochlorination reaction:

$$\underset{\text{dichlorohydrin}}{C_3H_6Cl_2O(l)} + \underset{\text{sodium hydroxide}}{NaOH(aq)} \longrightarrow \underset{\text{epichlorohydrin}}{C_3H_5ClO(l)} + \underset{\text{sodium chloride}}{NaCl(aq)} + \underset{\text{water}}{H_2O(l)}$$

Motivation is to create a more sustainable, efficient solution that maximizes profit, adheres to chemical engineering principles, and environmental standards

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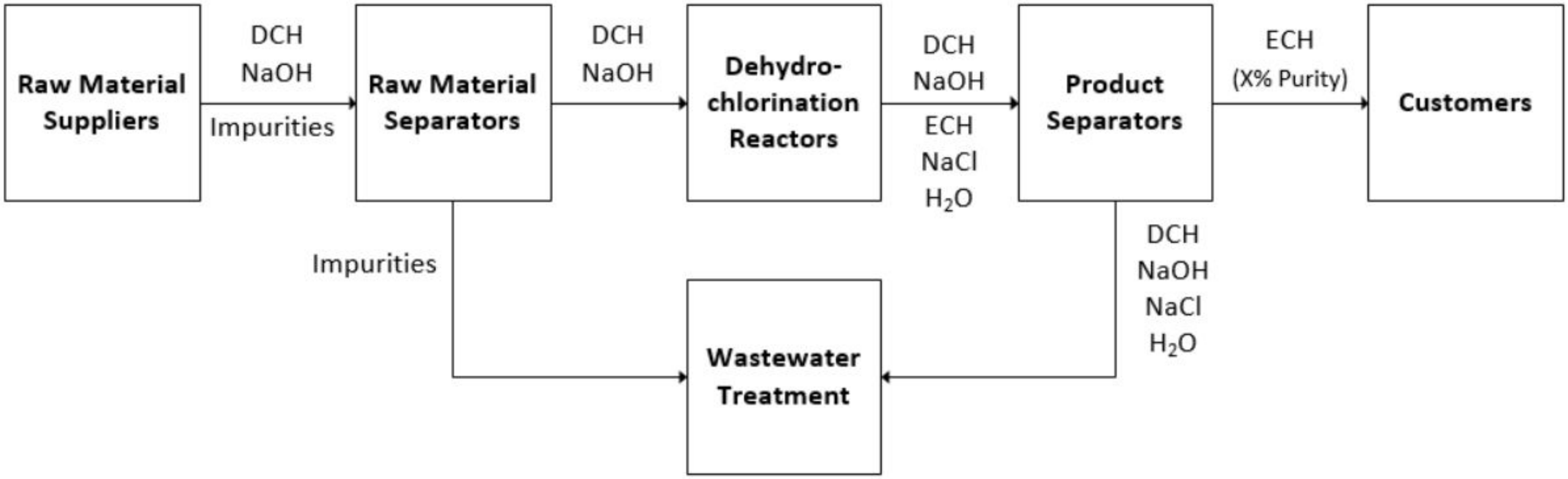
Block Flow Diagram



Data for Problem

Suppliers

- Unit cost of purchasing
- Varying levels of impurity
- Supply of a specific raw material

Separators

- Both fixed and unit cost
- 100% recovery for raw materials
- Varying recoveries for product streams

Reactors

- Both fixed and unit cost
- Different conversion rates
- Capacity of vessels

Customers

- Unit revenue
- Storage capacity
- Purity requirement

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Method to Solve

1,138 constraints
470 continuous and
40 binary variables

- Flow and Mass Conservation:

$$\sum_{m=1}^{M}\sum_{p=1}^{2} b_{mr}^{p} = \sum_{s=1}^{S}\sum_{p=1}^{P} d_{rs}^{p}\ , \quad \forall r \in R$$

- Costs:

$$UC_r = \sum_{p=1}^{P}\sum_{m=1}^{M}\sum_{r=1}^{R} c_r \times b_{mr}^{p} \qquad FC_r = \sum_{r=1}^{R} f_r \times \sigma_r \qquad \begin{array}{l} b_{mr}^{p} \leq \mathbf{M} \times \sigma_r \\ d_{rs}^{p} \leq \mathbf{M} \times \sigma_r \end{array}$$

- Separator Recovery:

$$\sum_{r=1}^{R} I_s \times d_{rs}^{p} = \sum_{l=1}^{L} \Delta e_{sl}^{p}\ , \quad \forall s \in S, \forall p \in \{1,2,3,4\}$$

- DCH Limiting Reactant:

$$\frac{\sum_{m=1}^{M} b_{mr}^{1}}{MW_{p=1}} \leq \frac{\sum_{m=1}^{M} b_{mr}^{2}}{MW_{p=2}}$$

Method to Solve

1,138 constraints
470 continuous and
40 binary variables

- NaOH Conversion:

$$\sum_{m=1}^{M} MW_{p=2} \times \left(\frac{b_{mr}^{p=2}}{MW_{p=2}} - \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}\right) = \sum_{s=1}^{S} d_{rs}^{p=2}$$

- Organic Waste Disposal:

$$\sum_{s=1}^{S} \Delta e_{sl}^{1} \leq 0.05 \times \sum_{s=1}^{S}\sum_{p=1}^{P} \Delta e_{sl}^{p}, \quad \forall l \in L$$

- Customer Demand:

$$\sum_{s=1}^{S}\sum_{p=1}^{P} e_{sk}^{p} \leq g_k, \quad \forall k \in K \qquad e_{sk}^{p} \leq \mathbf{M} \times e_{sk}^{5}$$

$$(1-\nu_k) \times \sum_{s=1}^{S}\sum_{p=1}^{P} e_{sk}^{p} \leq \sum_{s=1}^{S} e_{sk}^{5}, \quad \forall k \in K$$

Key Findings

Financial Success

$7.5M in Net Profit

$12.7M in Operating Cost

$20.2M in Sales Revenue

Option Utilization

4 separators and **2** reactors used

1 customer at storage capacity

4 distinct suppliers

Environmental Waste

$774K in aqueous waste

$143K in organic waste

8K MT waste

Impact & Conclusion

Optimization helps create sustainable and profitable solution

7.5M USD
net profit

- Maximize profit while maintaining sustainability
- Future Plant Improvement: Recycle more material instead of sending to wastewater
- Explore changes that allow scaling up to use all available capital

Conclusion: With optimization driven strategy, the plant is an environmentally and financially lucrative investment.

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Thank you!

Questions?

Appendix Slides

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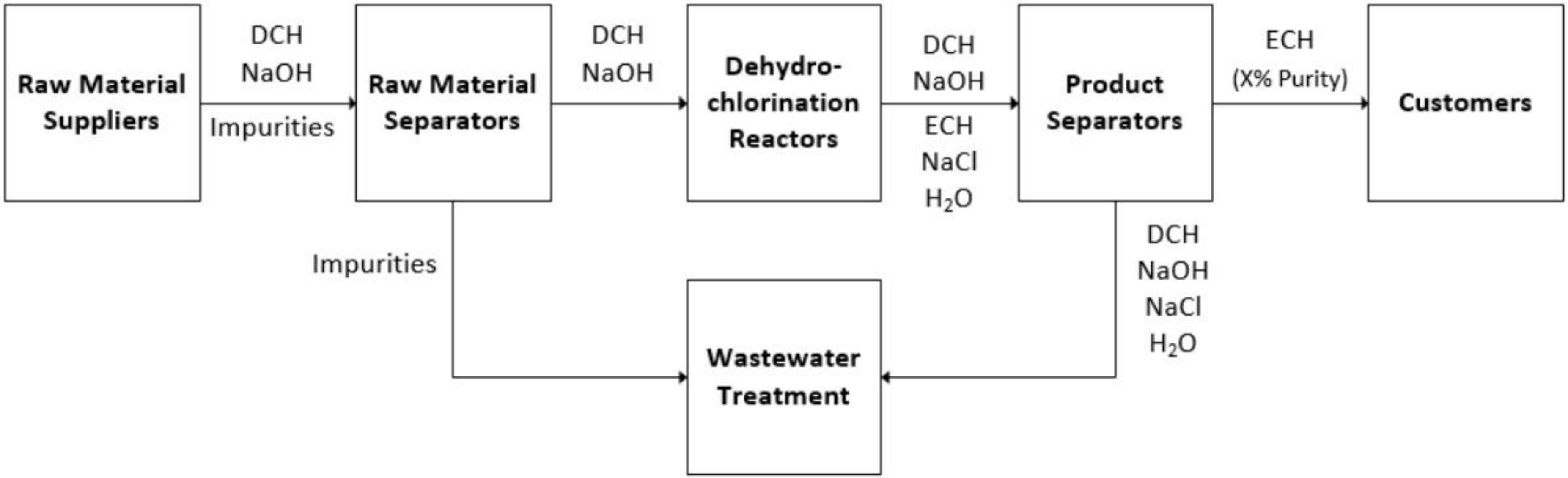
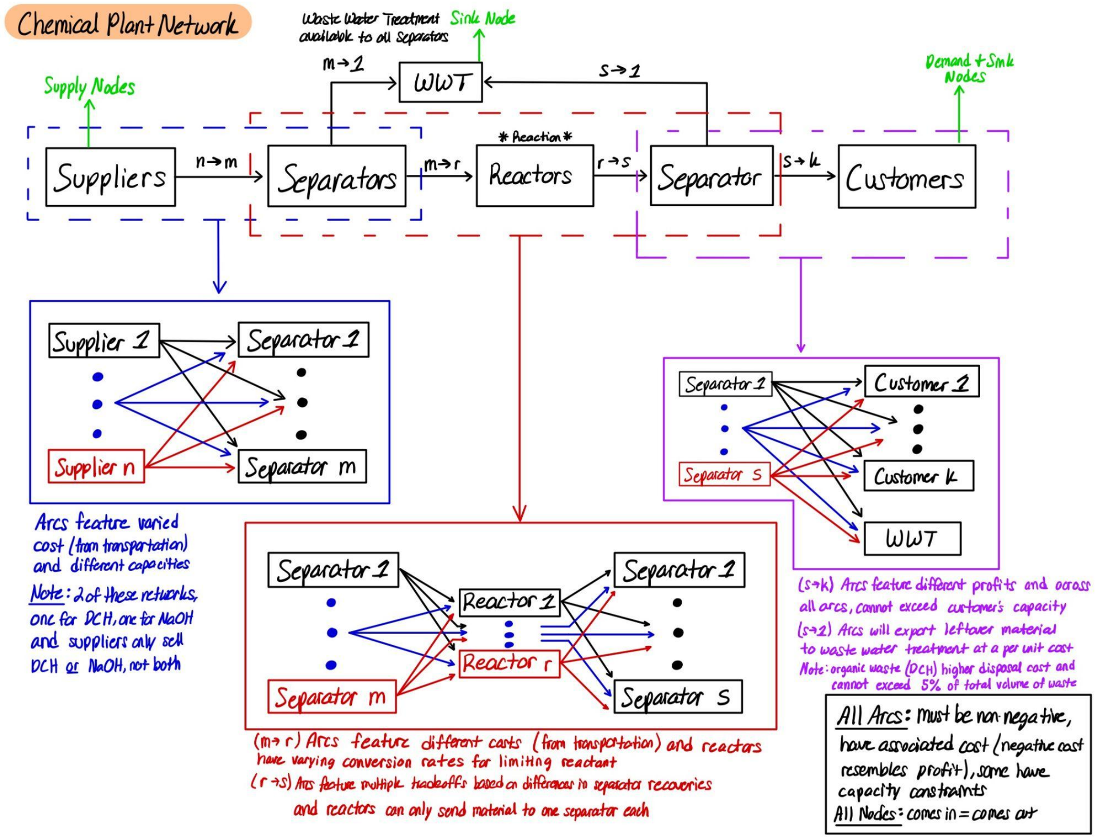
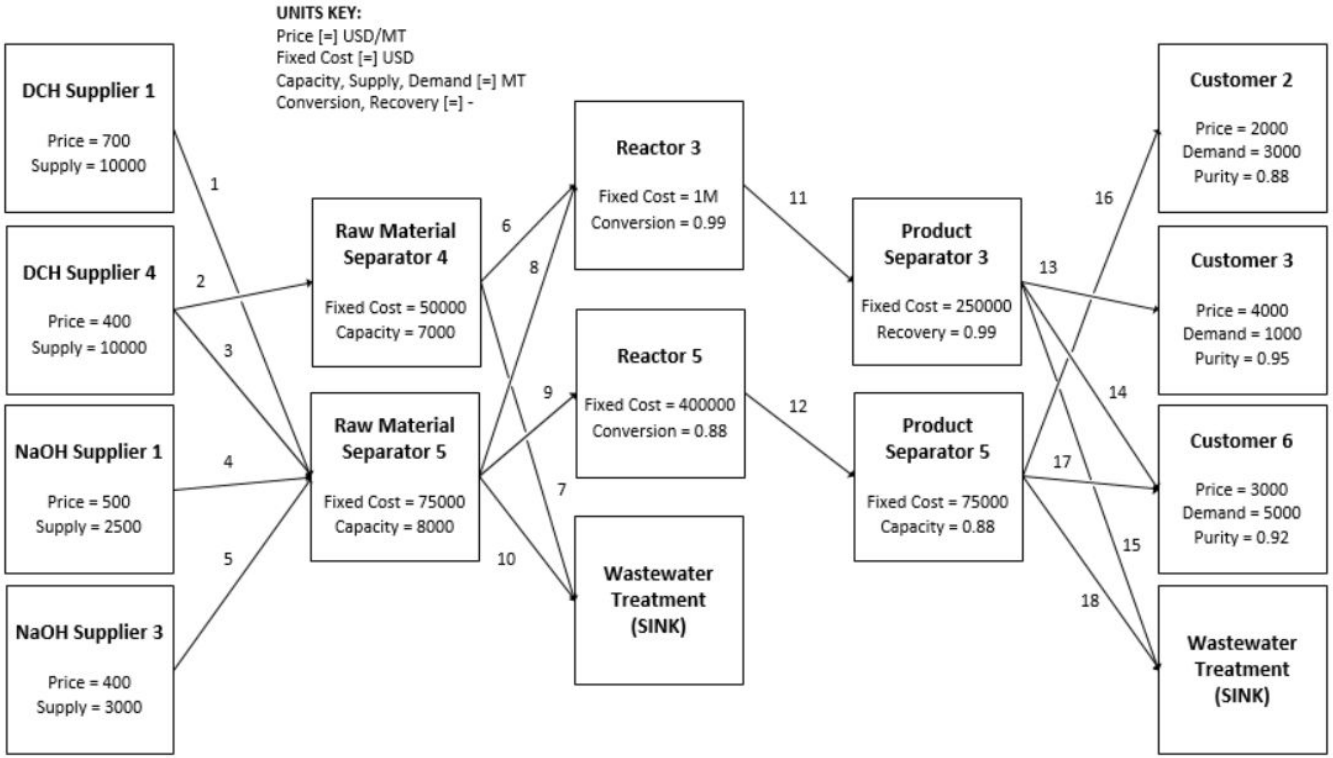
Flow of Chemicals in Plant



Network Representation of Chemical Plant



Solution


UNITS KEY:
Price [=] USD/MT
Fixed Cost [=] USD
Capacity, Supply, Demand [=] MT
Conversion, Recovery [=] -
DCH Supplier 1
Price = 700
Supply = 10000
DCH Supplier 4
Price = 400
Supply = 10000
NaOH Supplier 1
Price = 500
Supply = 2500
NaOH Supplier 3
Price = 400
Supply = 3000
Raw Material Separator 4
Fixed Cost = 50000
Capacity = 7000
Raw Material Separator 5
Fixed Cost = 75000
Capacity = 8000
Reactor 3
Fixed Cost = 1M
Conversion = 0.99
Reactor 5
Fixed Cost = 400000
Conversion = 0.88
Wastewater Treatment (SINK)
Product Separator 3
Fixed Cost = 250000
Recovery = 0.99
Product Separator 5
Fixed Cost = 75000
Capacity = 0.88
Customer 2
Price = 2000
Demand = 3000
Purity = 0.88
Customer 3
Price = 4000
Demand = 1000
Purity = 0.95
Customer 6
Price = 3000
Demand = 5000
Purity = 0.92
Wastewater Treatment (SINK)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18

Solution

Streams	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
DCH Flow [MT]	1713	7000	3000	0	0	5600	0	2033	1995	0	76	239	0	1	76	0	29	211
NaOH Flow [MT]	0	0	0	206	3000	0	0	2367	619	0	24	74	0	1	23	0	9	65
NaCl Flow [MT]	0	0	0	0	0	0	0	0	0	0	3424	795	0	34	3390	77	18	700
H_2O Flow [MT]	0	0	0	0	0	0	0	0	0	0	1055	245	0	11	1044	29	0	216
ECH Flow [MT]	0	0	0	0	0	0	0	0	0	0	5421	1259	1000	4421	0	781	478	0
Impure Flow [MT]	0	0	0	0	0	0	1400	0	0	906	0	0	0	0	0	0	0	0
Total Flow [MT]	1713	7000	3000	206	3000	5600	1400	4400	2614	906	10000	2612	1000	4468	4533	887	534	1192
Unit Cost [USD/MT]	45	35	45	45	45	200	100	200	85	100	50	50	-	-	Varies	-	-	Varies

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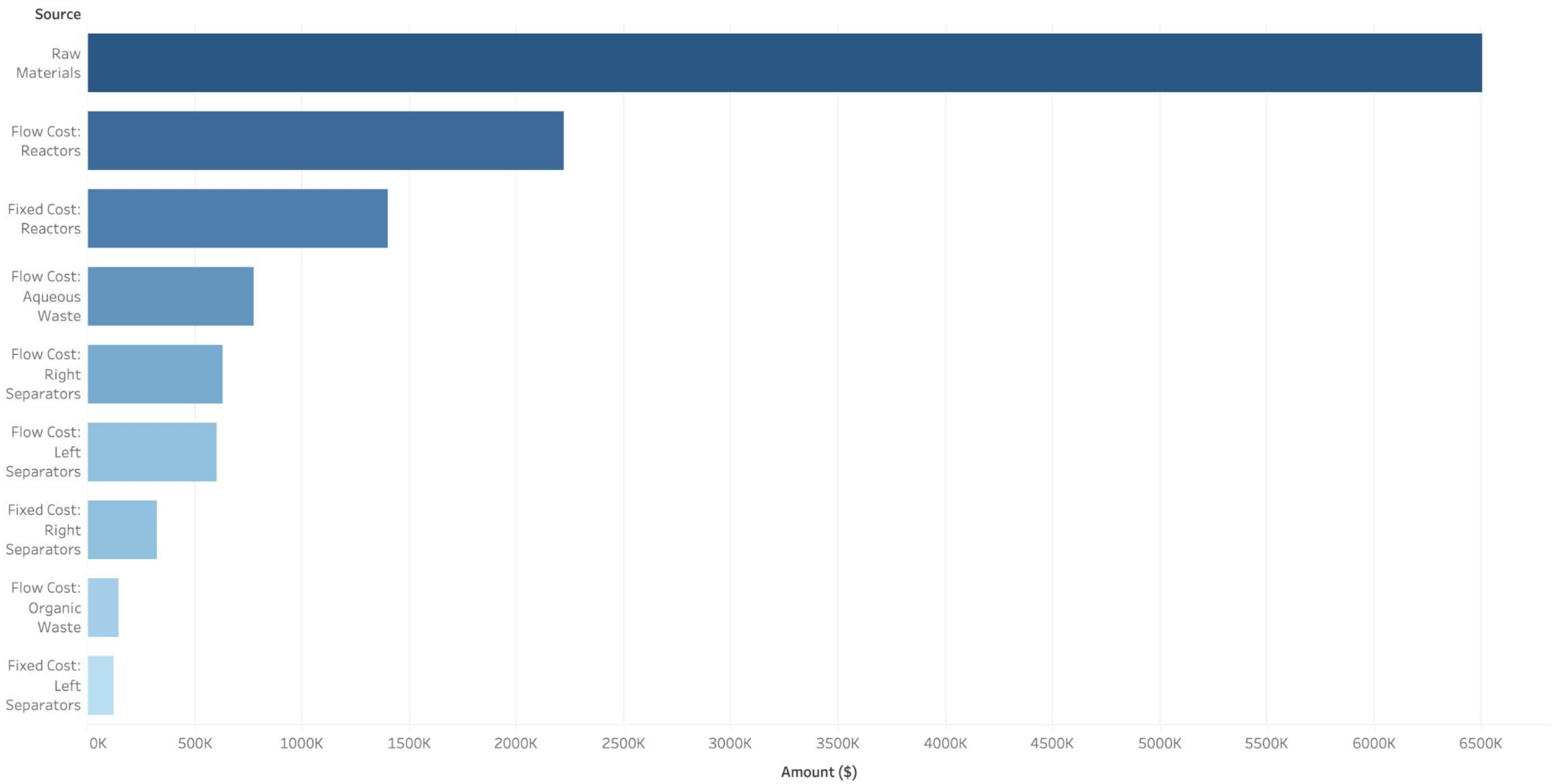
Solution


Source
Raw Materials
Flow Cost: Reactors
Fixed Cost: Reactors
Flow Cost: Aqueous Waste
Flow Cost: Right Separators
Flow Cost: Left Separators
Fixed Cost: Right Separators
Flow Cost: Organic Waste
Fixed Cost: Left Separators
0K
500K
1000K
1500K
2000K
2500K
3000K
3500K
4000K
4500K
5000K
5500K
6000K
6500K
Amount ($)

Cost Breakdown of Optimal Solution

Source	
Raw Materials	6,502,257
Flow Cost: Reactors	2,222,124
Fixed Cost: Reactors	1,400,000
Flow Cost: Aqueous Waste	774,383
Flow Cost: Right Separators	630,600
Flow Cost: Left Separators	601,363
Fixed Cost: Right Separators	325,000
Flow Cost: Organic Waste	143,102
Fixed Cost: Left Separators	125,000

Sets and Ranges for Problem

Sets of Values:

$$\text{Supplier } (n) \in [1, N]$$
$$\text{Material } (p) \in [1, P]$$
$$p = 1 \text{ for DCH}, p = 2 \text{ for NaOH}, p = 3 \text{ for NaCl}, p = 4 \text{ for H2O, and } p = 5 \text{ ECH}$$
$$\text{Separator (Left) } (m) \in [1, M]$$
$$\text{Waste Water Treatment Plant (for initial separators) } (j) \in [J]$$
$$\text{Reactors } (r) \in [1, R]$$
$$\text{Separator (Right) } (s) \in [1, S]$$
$$\text{Customers } (k) \in [1, K]$$
$$\text{Waste Water Treatment Plant (for second separators) } (l) \in [L]$$
$$\text{Aqueous Materials } (p \in \{2, 3, 4, 5\})$$
$$\text{Organic Materials } (p = 1)$$

$$\text{Fixed Cost for using separator (left) } (m) = f_m$$
$$\text{Fixed Cost for using reactor } (r) = f_r$$
$$\text{Fixed Cost for using separator (right) } (s) = f_s$$

$$\text{Unit Cost for sending material to separator (left) } (m) = c_m$$
$$\text{Unit Cost for sending material to waste water treatment plant } (j) = c_j$$
$$\text{Unit Cost for sending material to reaction } (r) = c_r$$
$$\text{Unit Cost for sending material to separator (right) } (s) = c_s$$
$$\text{Unit Cost for sending material to waste water treatment plant (aqueous) } (l) = c_l^A$$
$$\text{Unit Cost for sending material to waste water treatment plant (organic) } (l) = c_l^O$$
$$\text{Unit Profit for sending material to customer } k = p_k$$

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Variables in Model

$$
\begin{aligned}
a^p_{nm} \in \mathbb{R}_+ &= \text{amount of material } p \in \{1,2\} \text{ purchased from supplier } n \text{ and sent to separator } m \\
I_n &= \%\text{ impurity in material } p \in \{1,2\} \text{ purchased from supplier } n
\end{aligned}
$$

$$
\begin{aligned}
b^p_{mr} \in \mathbb{R}_+ &= \text{amount of separated (pure) material } p \in \{1,2\} \text{ to send from separator } m \text{ to reactor } r \\
\Delta b^p_{mj} \in \mathbb{R}_+ &= \text{amount of separated (impure) material } p \in \{1,2\} \text{ to send from separator } m \text{ to waste plant } j
\end{aligned}
$$

$$
\begin{aligned}
d^p_{rs} \in \mathbb{R}_+ &= \text{amount of reacted material } p \text{ (with impurities) to ship from reactor } r \text{ to separator } s \\
\gamma_r &= \%\text{ yield during reaction from reactor } r
\end{aligned}
$$

$$
\begin{aligned}
e^p_{sk} \in \mathbb{R}_+ &= \text{amount of separated material } p \text{ (pure) to ship from separator } s \text{ to customer } k \\
\Delta e^A_{sl} \in \mathbb{R}_+ &= \text{amount of separated (impure) aqueous material to ship from separator } s \text{ to waste plant } l \\
\Delta e^O_{sl} \in \mathbb{R}_+ &= \text{amount of separated (impure) organic material to ship from separator } s \text{ to waste plant } l \\
I_s &= \%\text{ recovery of materials from separator } s
\end{aligned}
$$

$$
\begin{aligned}
g_k \in \mathbb{R}_+ &= \text{units of demand from customer k} \\
\nu_k &= \text{maximum } \%\text{ of non-ECH product that customer } k \text{ willing to except, relative to amount of ECH shipped}
\end{aligned}
$$

$$
\begin{aligned}
\rho_m \in \{0,1\} &= \text{binary indicator if separator (left) } m \text{ used} \\
\sigma_r \in \{0,1\} &= \text{binary indicator if reactor } r \text{ used} \\
\mu_s \in \{0,1\} &= \text{binary indicator if separator (right) } s \text{ used} \\
z_{rs} \in \{0,1\} &= \text{binary indicator if reactor } r \text{ ships material to separator (right) } s
\end{aligned}
$$

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Conservation of Flow & Mass

$$\sum_{n=1}^{N} a^{p}_{nm} = \sum_{j=1}^{J} \Delta b^{p}_{mj} + \sum_{r=1}^{R} b^{p}_{mr} \,, \quad \forall p \in \{1,2\}, \forall m \in M, \forall j \in J$$

$$\sum_{m=1}^{M} \sum_{p=1}^{2} b^{p}_{mr} = \sum_{s=1}^{S} \sum_{p=1}^{P} d^{p}_{rs} \,, \quad \forall r \in R$$

$$\sum_{r=1}^{R} d^{p}_{rs} = \sum_{l=1}^{L} \Delta e^{p}_{sl} + \sum_{k=1}^{K} e^{p}_{sk} \,, \quad \forall s \in S, \forall p \in P$$

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Fixed Cost for Primary (Left) Separators

$$a^{p}_{nm} \leq \mathbf{M} \times \rho_m \;, \quad \forall n \in N, \forall p \in P, \forall m \in M$$

$$b^{p}_{mr} \leq \mathbf{M} \times \rho_m \;, \quad \forall p \in P, \forall m \in M, \forall r \in R$$

$$\Delta b^{p}_{mj} \leq \mathbf{M} \times \rho_m \;, \quad \forall p \in P, \forall m \in M, \forall j \in J$$

$$FC_m = \sum_{m=1}^{M} f_m \times \rho_m$$

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Fixed Cost for Reactors

$$b_{mr}^{p} \leq \mathbf{M} \times \sigma_r \,, \qquad \forall p \in P, \forall m \in M, \forall r \in R$$

$$d_{rs}^{p} \leq \mathbf{M} \times \sigma_r \,, \qquad \forall r \in R, \forall p \in P, \forall s \in S$$

$$FC_r = \sum_{r=1}^{R} f_r \times \sigma_r$$

Fixed Cost for Secondary (Right) Separators

$$d^p_{rs} \leq \mathbf{M} \times \mu_s \,, \quad \forall r \in R, \forall p \in P, \forall s \in S$$

$$e^p_{sk} \leq \mathbf{M} \times \mu_s \,, \quad \forall s \in S, \forall p \in P, \forall k \in K$$

$$\Delta e^p_{sl} \leq \mathbf{M} \times \mu_s \,, \quad \forall s \in S, \forall p \in P, \forall l \in L$$

$$FC_s = \sum_{s=1}^{S} f_r \times \mu_s$$

Customer Demand Constraints

$$\sum_{s=1}^{S}\sum_{p=1}^{P} e_{sk}^{p} \leq g_k \,, \quad \forall k \in K$$

$$(1-\nu_k) \times \sum_{s=1}^{S}\sum_{p=1}^{P} e_{sk}^{p} \leq \sum_{s=1}^{S} e_{sk}^{5} \,, \quad \forall k \in K$$

$$e_{sk}^{p} \leq \mathbf{M} \times e_{sk}^{5} \,, \quad \forall s \in S, \forall k \in K, \forall p \in \{1,2,3,4\}$$

Unit Cost Calculations

$$UC_n = \sum_{p=1}^{P}\sum_{n=1}^{N}\sum_{m=1}^{M} c_n \times a_{nm}^{p}$$

$$UC_m = \sum_{p=1}^{P}\sum_{n=1}^{N}\sum_{m=1}^{M} c_m \times a_{nm}^{p}$$

$$UC_j = \sum_{p=1}^{P}\sum_{m=1}^{M}\sum_{j=1}^{J} c_j \times \Delta b_{mj}^{p}$$

$$UC_r = \sum_{p=1}^{P}\sum_{m=1}^{M}\sum_{r=1}^{R} c_r \times b_{mr}^{p}$$

$$UC_s = \sum_{p=1}^{P}\sum_{r=1}^{R}\sum_{s=1}^{S} c_s \times d_{rs}^{p}$$

$$UC_l = \sum_{s=1}^{S}\sum_{l=1}^{L}(c_l^{A} \times \Delta e_{sl}^{A} + c_l^{O} \times \Delta e_{sl}^{O})$$

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Arc Flow Capacities

$$\sum_{m=1}^{M} a_{nm}^{p} \leq supply_N \,, \quad \forall n \in N, \forall p \in \{1,2\}$$

$$\sum_{n=1}^{N} \sum_{p=1}^{2} a_{nm}^{p} \leq capacity_M \,, \quad \forall m \in M$$

$$\sum_{j=1}^{J} \Delta b_{mj}^{p} + \sum_{r=1}^{R} \sum_{p=1}^{2} b_{mr}^{p} \leq capacity_M \,, \quad \forall m \in M$$

$$\sum_{m=1}^{M} \sum_{p=1}^{2} b_{mr}^{p} \leq capacity_R \,, \quad \forall r \in R$$

$$\sum_{s=1}^{S} \sum_{p=1}^{2} d_{rs}^{p} \leq capacity_R \,, \quad \forall r \in R$$

$$\sum_{r=1}^{R} \sum_{p=1}^{P} d_{rs}^{p} \leq capacity_S \,, \quad \forall s \in S$$

$$\sum_{l=1}^{L} \sum_{p=1}^{P} \Delta e_{sl}^{p} + \sum_{p=1}^{P} \sum_{k=1}^{K} e_{sk}^{p} \leq capacity_S \,, \quad \forall s \in S$$

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Recovery from Primary (Left) Separators

$$\sum_{n=1}^{N}(1 - I_n) \times a_{nm}^{p} = \sum_{r=1}^{R} b_{mr}^{p} \,, \quad \forall m \in M, \forall p \in \{1,2\}$$

$$\sum_{n=1}^{N} I_n \times a_{nm}^{p} = \sum_{j=1}^{J} \Delta b_{mj}^{p} \,, \quad \forall m \in M, \forall p \in \{1,2\}$$

Chemical Conversion Calculations for Reactors

$$\sum_{m=1}^{M} MW_{p=1} \times (\frac{b_{mr}^{p=1}}{MW_{p=1}} - \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}) = \sum_{s=1}^{S} d_{rs}^{p=1}, \quad \forall r \in R$$

$$\sum_{m=1}^{M} MW_{p=2} \times (\frac{b_{mr}^{p=2}}{MW_{p=2}} - \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}) = \sum_{s=1}^{S} d_{rs}^{p=2}, \quad \forall r \in R$$

$$\sum_{m=1}^{M} (MW_{p=3} \times \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}) = \sum_{s=1}^{S} d_{rs}^{p=3}, \quad \forall r \in R$$

$$\sum_{m=1}^{M} (MW_{p=4} \times \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}) = \sum_{s=1}^{S} d_{rs}^{p=4}, \quad \forall r \in R$$

$$\sum_{m=1}^{M} (MW_{p=5} \times \gamma_r \times \frac{b_{mr}^{p=1}}{MW_{p=1}}) = \sum_{s=1}^{S} d_{rs}^{p=5}, \quad \forall r \in R$$

Recovery from Secondary (Right) Separators

$$\sum_{r=1}^{R} I_s \times d_{rs}^{p} = \sum_{l=1}^{L} \Delta e_{sl}^{p} \,, \quad \forall s \in S, \forall p \in \{1,2,3,4\}$$

$$\sum_{r=1}^{R} d_{rs}^{5} = \sum_{k=1}^{K} e_{sk}^{5} \,, \quad \forall s \in S$$

$$\sum_{r=1}^{R} (1 - I_s) \times d_{rs}^{p} = \sum_{k=1}^{K} e_{sk}^{p} \,, \quad \forall s \in S, \forall p \in \{1,2,3,4\}$$

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Requirements for Organic Waste Disposal

$$\sum_{s=1}^{S} \Delta e_{sl}^{1} \leq 0.05 \times \sum_{s=1}^{S} \sum_{p=1}^{P} \Delta e_{sl}^{p}, \quad \forall l \in L$$

DCH (p=1) is the Limiting Reactant

$$\frac{\sum_{m=1}^{M} b_{mr}^{1}}{MW_{p=1}} \leq \frac{\sum_{m=1}^{M} b_{mr}^{2}}{MW_{p=2}}, \quad \forall r \in R$$

Rector Flow Remains Together

$$\sum_{s=1}^{S} z_{rs} \leq 1 \,, \quad \forall r \in R$$

$$z_{rs} \leq \mu_s \,, \quad \forall r \in R, \forall s \in S$$

$$z_{rs} \leq \sigma_r \,, \quad \forall r \in R, \forall s \in S$$

$$d_{rs}^{p} \leq \mathbf{M} \times z_{rs} \,, \quad \forall r \in R, \forall s \in S, \forall p \in P$$

Revenue Calculation & Objective Function

$$R_k = \sum_{s=1}^{S} \sum_{k=1}^{K} p_k \times e_{sk}^{5}$$

$$\max \quad R_k - (UC_n + FC_m + UC_m + FC_r + UC_r + FC_s + UC_s + UC_j + UC_l)$$