Optimization in Application: Green Epichlorohydrin Plant Production

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15.093 - Optimization Methods
December 8, 2023

Problem & Reasoning

Epichlorohydrin (ECH) is a key intermediate in the production of epoxy resins, which are used in a large variety of products such as adhesives, electronics, and protective coatings. ECH has historically been produced using petroleum-derived byproducts, but recent research has demonstrated that ECH can also be produced using a glycerol-derived pathway. Glycerol is a major byproduct of the rapidly growing biodiesel industry, so glycerol processes are considered more environmentally friendly. The goal was to optimize a plant that produces glycerol-derived ECH for financial and environmental benefits. The general pathway is:

$$\text{Glycerol} \rightarrow \text{DCH} \rightarrow \text{ECH}$$

For simplicity, the analysis only focused on the second step of the pathway (DCH→ECH). The dehydrochlorination reaction that converts DCH to ECH is:

$$DCH + NaOH \rightarrow ECH + NaCl + H_2O$$

Figure 1 shows the basic structure of the plant, and Figure 2 shows the plant represented as a network. Both figures are presented in the Appendix.

There are two sets of raw material suppliers, one for DCH and one for NaOH. Each supplier offers a unique price, amount of material, and percent impurity, which is the percentage of the supply that is impure.

Separators are needed to remove the impurities in the raw material streams. These separators achieve perfect separation, but they vary in transportation costs, fixed costs, and capacity. The higher-cost separators are able to process more material. The impurities are perfectly removed and sent to wastewater treatment. Wastewater treatment has an associated flow cost.

The purified DCH and NaOH streams are then sent to reactors to carry out the dehydrochlorination reactions. Each reactor varies in fixed costs, transportation costs, and achievable conversion (amount of limiting reactant converted into products). The higher-cost reactors achieve a higher conversion. Since no reactor achieves 100% conversion, the outlet streams from the reactors contain unreacted reactants (DCH and NaOH), byproducts (NaCl and H_2O), and the desired product ECH.

The reactor outlet streams are then sent to separators to purify the product ECH for the customers. Each separator varies in fixed costs and percent recovery (the percentage of the unreacted reactants and byproducts removed from the ECH stream). The higher-cost separators achieve a higher level of ECH purity. The unreacted reactants and byproducts are sent to wastewater treatment. It is assumed that wastewater can not be more than 5% organic to prevent environmental damage, so the amount of DCH in wastewater must be limited. Additionally, organics in wastewater have a larger unit cost than aqueous species.

The purified ECH streams are then sent to customers. Each customer has purity requirements and is charged a unique price per unit. The higher-paying customers require higher purities. The customers have storage capacity constraints, so they can not receive more than their requested amount. There are no demand requirements.

Data for Problem

All cost data is synthetic, with some estimates derived from real-world values. For example, the prices paid by customers vary closely around ECH's price in November 2018, which was 1840 USD/metric ton (Intratec). Additionally, several constraints are synthetic, such as the constraint that wastewater's organic composition can not exceed 5%. Most of the physical and chemical property data, such as molecular weights and stoichiometric coefficients, are based on actual measurements. However, separator recoveries and reaction conversions are synthetic. Tables 1-8 in the Appendix display the individual data tables used by the optimization model.

Method to Solve

A mixed-integer optimization (MIO) formulation was developed to maximize the plant's profit. The full formulation is presented in the Appendix (Figures 5-21). The underlying design of the model follows a network/graph structure. Network structures are powerful ways to linearly represent the flow of materials and assignment of resources between nodes, much like a true chemical plant would do.

The primary decisions are the amount of DCH and NaOH to purchase from suppliers, which separators and reactors to use, how much flow to allocate to each separator and reactor, and the amount of product ECH to send to each customer. The most significant constraints are discussed herein.

By the Law of Conservation of Mass, the total amount of mass entering a specific node must equal the total amount of mass exiting the node (Equation 1). This ensures the plant runs continuously without accumulation of material.

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

Equation 1: Total mass of materials entering reactor must exit reactor

The cost incurred by the plant consists of unit/flow costs and fixed costs (Equations 2 and 3). The objective function includes these values to calculate net profit, which the model aims to maximize.

$$FC_r = \sum_{r=1}^{R} f_r \times \sigma_r \quad \begin{array}{ll} b_{mr}^{p} \leq \mathbf{M} \times \sigma_r \ , & \forall p \in P, \forall m \in M, \forall r \in R \\ d_{rs}^{p} \leq \mathbf{M} \times \sigma_r \ , & \forall r \in R, \forall p \in P, \forall s \in S \end{array}$$

Equation 2: Fixed-cost (f_r) if reactor r processes any material

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

Equation 3: Unit of processing product through reactor r

Each product separator has a percent recovery I_s that determines how well it removes the unreacted reactants and byproducts from the product stream (Equation 4)

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

Equation 4: Recovery from product separators, in terms of unreacted reactants and byproducts

To preemptively reduce operating and disposal costs, DCH is constrained to be the limiting reactant, which is the reactant with the least initial moles (Equation 5). Indeed, DCH costs significantly more than NaOH (Tables 2 and 3), and its disposal incurs higher wastewater costs since it is organic (Table 8). The molecular weight of a chemical, as represented by *MW*, is used to convert between molar and mass bases.

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

Equation 5: Moles of DCH (p = 1) cannot exceed the moles of NaOH (p = 2) for reactor r

By constraining DCH to be the limiting reactant, the proper chemical reaction equations can be enforced (Equation 6). The amount of material exiting a reactor is determined by the material's initial amount, the limiting reactant's initial amount, and the reactor's conversion. These calculations occur on a molar basis.

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

Equation 6: Chemical conversion equation for NaOH (p = 2), from reactor r with conversion γ_r

The following constraint limiting the amount of organic material in wastewater was added to comply with environmental regulations (Equation 7). As mentioned in the *Data for Problem* section, it was estimated that the wastewater's organic composition cannot exceed 5%. The only organic material sent to wastewater is DCH, which corresponds to p = 1.

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

Equation 7: Wastewater organic composition can not exceed 5%

The model treats each material as separate entities, not reflecting the real-world scenario where materials flow together as one solution. To ensure that this real-world behavior is not violated, the following constraint requires all flow exiting a reactor to move together (Equation 8). This constraint is overly restrictive, but the only alternative is a complex non-linear constraint that enforces a proportional dispersion of materials. This constraint is not required for separators since they are physically able to alter the composition of a solution. The binary variable 'z' selects one operational separator per reactor, with flow regulated by a 'big M' constraint.

$$\begin{aligned} &\sum_{s=1}^{S} z_{rs} \leq 1 \,, \quad \forall r \in R \\ &z_{rs} \leq \mu_s \,, \quad \forall r \in R, \forall s \in S \\ &z_{rs} \leq \sigma_r \,, \quad \forall r \in R, \forall s \in S \\ &d_{rs}^{p} \leq \mathbf{M} \times z_{rs} \,, \quad \forall r \in R, \forall s \in S, \forall p \in P \end{aligned}$$

Equation 8: Enforcing unified movement of materials from reactors to separators

To properly serve the plant's customer base, the material shipped to a customer cannot exceed their storage capacity (Equation 9) and must satisfy their purity requirement (Equation 10).

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

Equation 9: The amount of material sent to customer k cannot exceed g_k

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

Equation 10: Customer k requires ECH purity to be 1-ν_k

Key Findings

The plant is financially successful, achieving a profit of 7.5M USD. The sales revenue is 20.2M, and the total operating cost is 12.7M USD. Figure 3 in the Appendix provides a breakdown of the operating costs. The raw material costs are the most substantial by far, which is unsurprising considering ~11.7K and 3.2K metric tons of DCH and NaOH are purchased, respectively. Reactor costs are next most substantial, which is unsurprising considering they perform more complex unit operations than most other vessels, such as separators.

~8K metric tons of material are sent to wastewater, resulting in total waste costs of nearly 900K USD. This is certainly an area of improvement for the plant. As a cost-savings measure, some of the unreacted reactants and byproducts from the second set of separators could be recycled back to the reactor to increase yield and reduce waste costs.

Figure 3 and Table 9 in the Appendix display the solution. Interestingly, the optimal solution does not suggest using most of the available capital. The model selected only two out of the five units for the raw material separators, the reactors, and the product separators. As a result, only three customers out of six receive any ECH, and only one customer receives the full amount requested. Scaling up the plant to utilize more of the available capital would thus require greater efficiency or external factors to change, such as the unit price or demanded volume of ECH to increase.

Furthermore, the solution uses a mixture of low-cost and high-cost equipment. For example, the solution uses low-cost raw material separators with low capacities as well as a high-cost reactor with near-perfect conversion and a high-cost separator with near-perfect recovery. By using the high-cost reactors and product separators, the plant is able to serve the highest-paying customer, despite the requirement of 95% purity.

Conclusion

Optimizing a glycerol-derived ECH production plant has demonstrated significant financial and environmental benefits. Indeed, the mixed-integer model successfully found a solution that generates a profit of 7.5M USD, proving that this plant is a worthy candidate in the green glycerol pipeline. Still, waste management and scaling up are critical areas of operational improvement. Furthermore, by improving the model to more accurately capture chemical systems, the plant can further cement itself as an environmentally and financially lucrative investment.

Appendix

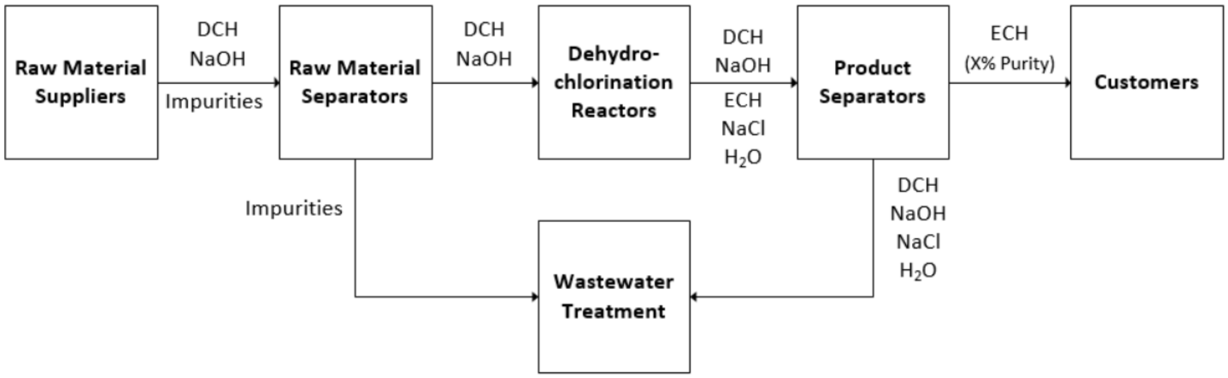

Figure 1: Basic Flow Diagram of Plant

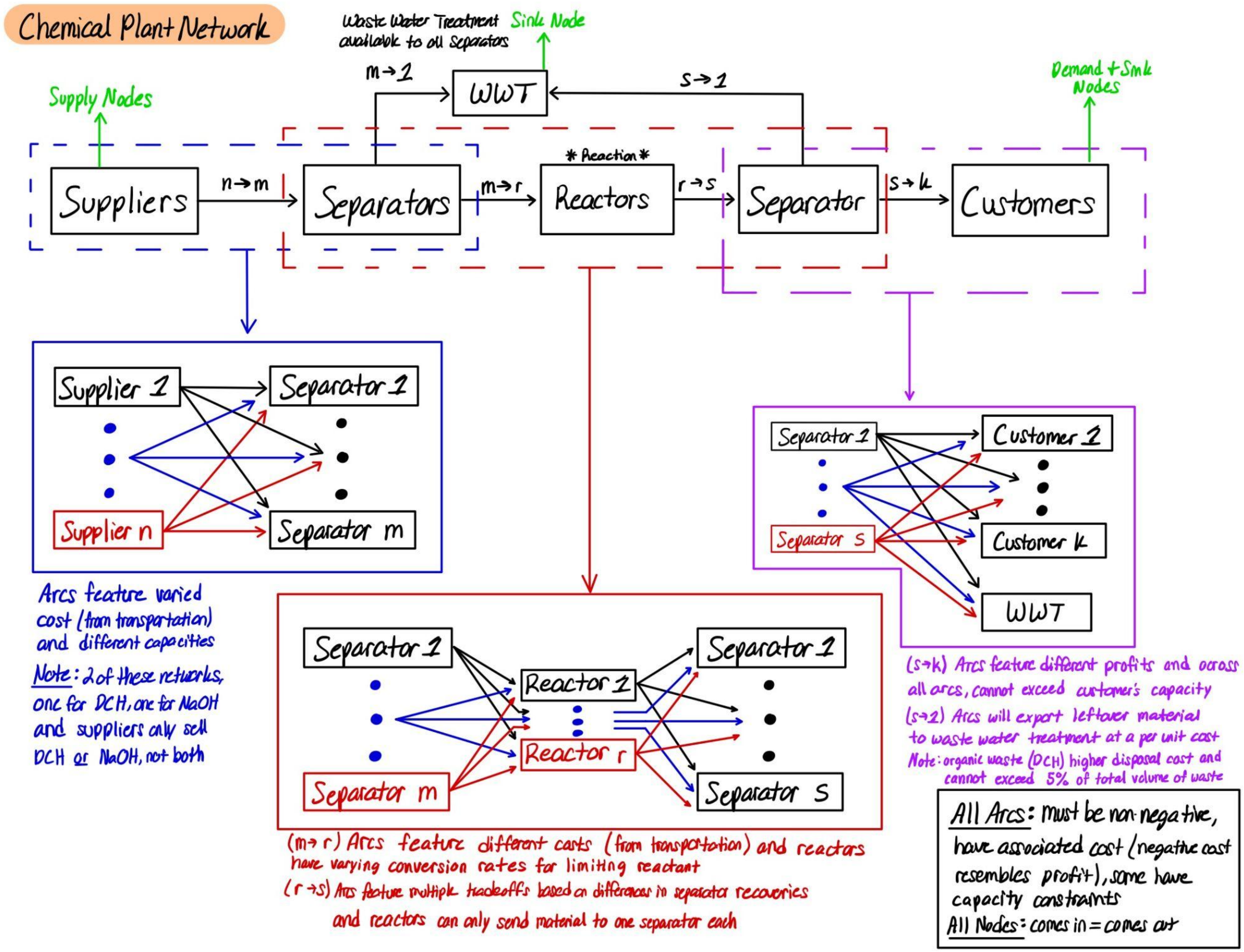

Figure 2: Network representation of plant

Table 1: Molecular weight and price of process chemicals.

Chemical	MW [MT/mol]	Price [USD/MT]
ECH	9.25E-05	1840
DCH	1.29E-04	700
NaOH	4.00E-05	492
H20	1.80E-05	-
NaCL	5.84E-05	-

Table 2: Availability and price of DCH suppliers.

Price [USD/MT]	Supply [MT]
700	10000
800	10000
1200	5000
400	10000
900	5000

Table 3: Availability and price of NaOH suppliers.

Price [USD/MT]	Supply [MT]
500	2500
600	2000
400	3000
1000	2000
800	2500

Table 4: Costs and capacities of raw material separators.

Fixed Cost [USD]	Flow Cost [USD/MT]	Capacity [MT]
100000	50	10000
200000	100	20000
250000	120	21000
50000	35	7000
75000	45	8000

Table 5: Costs, capacities, and conversions of reactors.

Fixed Cost [USD]	Flow Cost [USD/MT]	Capacity [MT]	Conversion [-]
500000	100	10000	0.9
800000	175	10000	0.95
1000000	200	10000	0.99
300000	80	10000	0.8
400000	85	10000	0.88

Table 6: Costs, capacities, and conversions of product separators.

Fixed Cost [USD]	Flow Cost [USD/MT]	Capacity [MT]	Recovery [-]
100000	50	10000	0.9
200000	50	10000	0.95
250000	50	10000	0.99
50000	50	10000	0.85

75000	50	10000	0.88

Table 7: Price, demand, and required purity of customers.

Price [USD/MT]	Demand [MT]	Purity [-]
1840	5000	0.15
2000	3000	0.12
4000	1000	0.05
1500	8000	0.14
1700	8000	0.17
3000	5000	0.08

Table 8: Aqueous and organic waste flow costs.

Aqueous Waste Flow Cost [USD/MT]	Organic Waste Flow Cost [USD/MT]
100	500

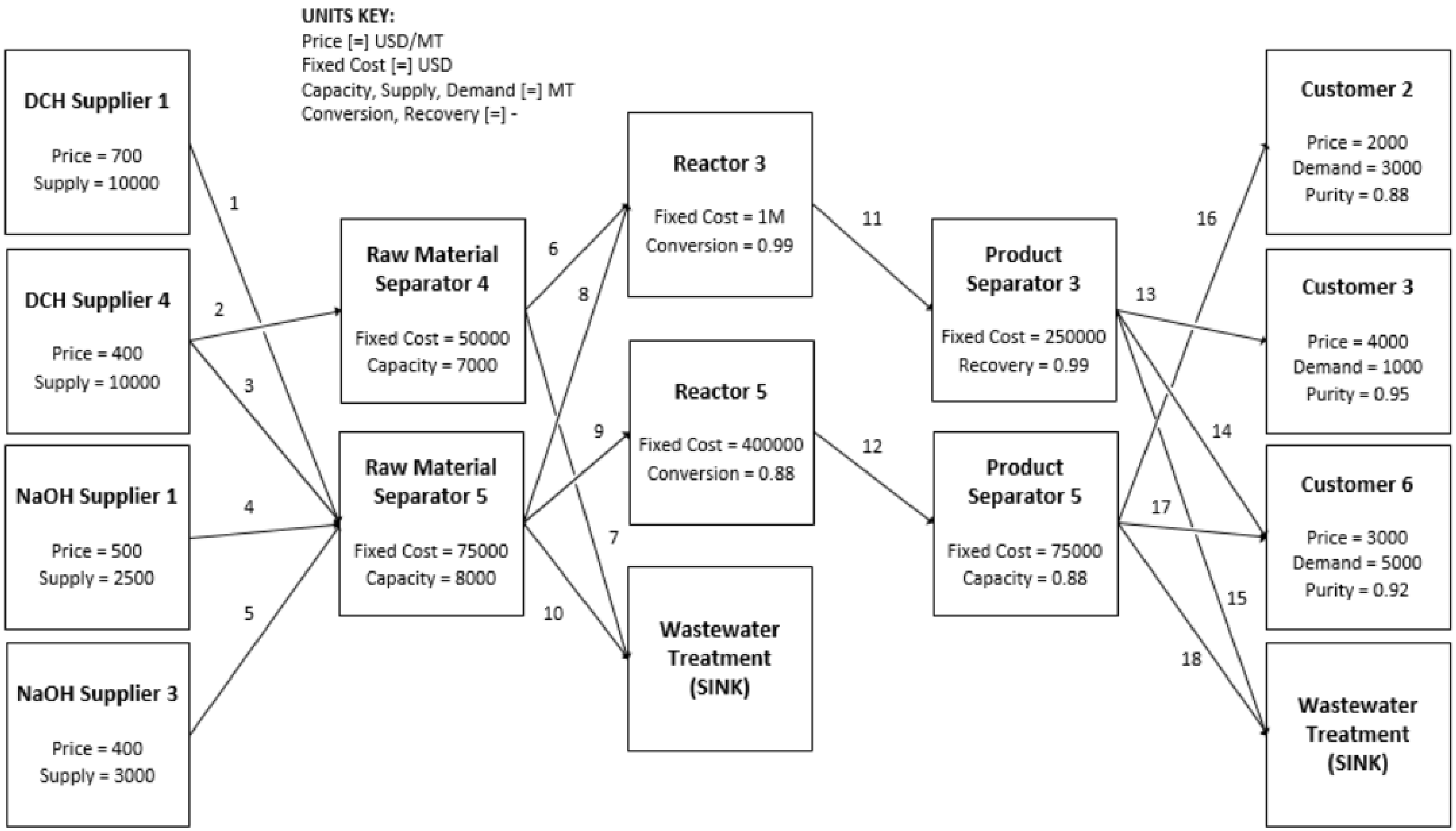

Figure 3: Characterization of Plant based on Optimal Solution; Stream Information Presented in Table 9

Table 9: Stream tables for optimal 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

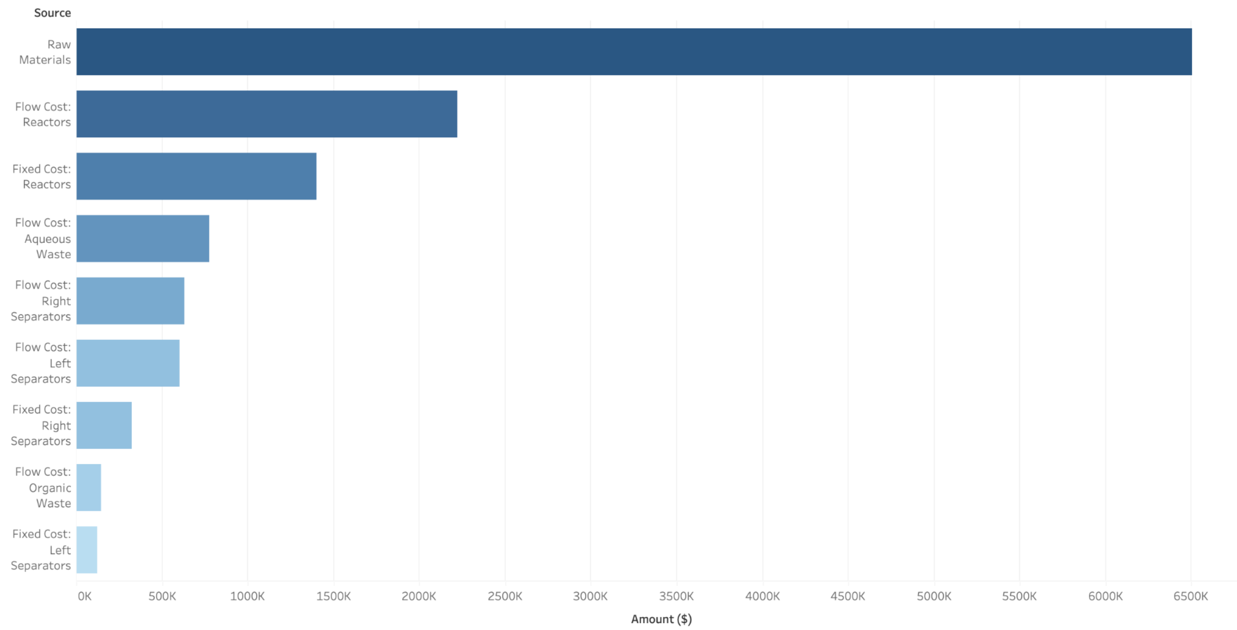

Figure 4: Cost Breakdown of Optimal Solution

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

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

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

Figure 5: Defining Formulation Sets and Ranges

$$
\begin{aligned}
a^p_{nm} \in \mathbb{R}_+ &= \text{amount of material } p \in \{1,2\} \text{ purchased from supplier } n \text{ and sent to separator } m \\
I_n &= \text{\% impurity in material } p \in \{1,2\} \text{ purchased from supplier } n \\
\\
b^p_{mr} \in \mathbb{R}_+ &= \text{amount of separated (pure) material } p \in \{1,2\} \text{ to send from separator } m \text{ to reactor } r \\
\Delta b^p_{mj} \in \mathbb{R}_+ &= \text{amount of separated (impure) material } p \in \{1,2\} \text{ to send from separator } m \text{ to waste plant } j \\
\\
d^p_{rs} \in \mathbb{R}_+ &= \text{amount of reacted material } p \text{ (with impurities) to ship from reactor } r \text{ to separator } s \\
\gamma_r &= \text{\% yield during reaction from reactor } r \\
\\
e^p_{sk} \in \mathbb{R}_+ &= \text{amount of separated material } p \text{ (pure) to ship from separator } s \text{ to customer } k \\
\Delta e^A_{sl} \in \mathbb{R}_+ &= \text{amount of separated (impure) aqueous material to ship from separator } s \text{ to waste plant } l \\
\Delta e^O_{sl} \in \mathbb{R}_+ &= \text{amount of separated (impure) organic material to ship from separator } s \text{ to waste plant } l \\
I_s &= \text{\% recovery of materials from separator } s \\
\\
g_k \in \mathbb{R}_+ &= \text{units of demand from customer k} \\
\nu_k &= \text{maximum \% of non-ECH product that customer } k \text{ willing to except, relative to amount of ECH shipped} \\
\\
\rho_m \in \{0,1\} &= \text{binary indicator if separator (left) } m \text{ used} \\
\sigma_r \in \{0,1\} &= \text{binary indicator if reactor } r \text{ used} \\
\mu_s \in \{0,1\} &= \text{binary indicator if separator (right) } s \text{ used} \\
z_{rs} \in \{0,1\} &= \text{binary indicator if reactor } r \text{ ships material to separator (right) } s
\end{aligned}
$$

Figure 6: Defining Decision Variables

$$
\begin{aligned}
&\sum_{n=1}^{N} a^p_{nm} = \sum_{j=1}^{J} \Delta b^p_{mj} + \sum_{r=1}^{R} b^p_{mr}\ , \quad \forall p \in \{1,2\}, \forall m \in M, \forall j \in J \\
&\sum_{m=1}^{M} \sum_{p=1}^{2} b^p_{mr} = \sum_{s=1}^{S} \sum_{p=1}^{P} d^p_{rs}\ , \quad \forall r \in R \\
&\sum_{r=1}^{R} d^p_{rs} = \sum_{l=1}^{L} \Delta e^p_{sl} + \sum_{k=1}^{K} e^p_{sk}\ , \quad \forall s \in S, \forall p \in P
\end{aligned}
$$

Figure 7: Conservation of Flow & Mass

$$a^p_{nm} \leq \mathbf{M} \times \rho_m \ , \quad \forall n \in N, \forall p \in P, \forall m \in M$$
$$b^p_{mr} \leq \mathbf{M} \times \rho_m \ , \quad \forall p \in P, \forall m \in M, \forall r \in R$$
$$\Delta b^p_{mj} \leq \mathbf{M} \times \rho_m \ , \quad \forall p \in P, \forall m \in M, \forall j \in J$$

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

Figure 8: Fixed Cost for Primary (Left) Separators

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

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

Figure 9: Fixed Cost for Reactors

$$d^p_{rs} \leq \mathbf{M} \times \mu_s \ , \quad \forall r \in R, \forall p \in P, \forall s \in S$$
$$e^p_{sk} \leq \mathbf{M} \times \mu_s \ , \quad \forall s \in S, \forall p \in P, \forall k \in K$$
$$\Delta e^p_{sl} \leq \mathbf{M} \times \mu_s \ , \quad \forall s \in S, \forall p \in P, \forall l \in L$$

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

Figure 10: Fixed Cost for Secondary (Right) Separators

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

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

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

Figure 11: Customer Demand Constraints

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

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

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

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

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

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

Figure 12: Unit Cost Calculations

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

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

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

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

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

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

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

Figure 13: Arc Flow Capacities

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

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

Figure 14: Recovery from Primary (Left) Separators

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

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

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

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

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

Figure 15: Chemical Conversion Calculations for Reactors

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

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

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

Figure 16: Recovery from Secondary (Right) Separators

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

Figure 17: Requirements for Organic Waste Disposal

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

Figure 18: DCH (p=1) is the Limiting Reactant

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

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

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

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

Figure 19: Rector Flow Remains Together

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

Figure 20: Revenue Calculation

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

Figure 21: Objective Function