

## Overview

This project focuses on the design of a small-scale chlor-alkali plant for the Baltimore area, producing approximately 25 tons/day of chlorine via membrane-based electrolysis of purified brine. The process converts sodium chloride and water into chlorine gas, hydrogen, and caustic soda (NaOH), followed by downstream separation, drying, compression, and liquefaction of chlorine for storage and transport. Hydrogen byproduct is recovered to be reacted with chlorine to produce hydrochloric acid, while caustic soda is concentrated for industrial use. The design emphasizes safe handling of hazardous chlorine, and sustainable operation through energy optimization and byproduct utilization, while integrating economic viability.

## Motivation

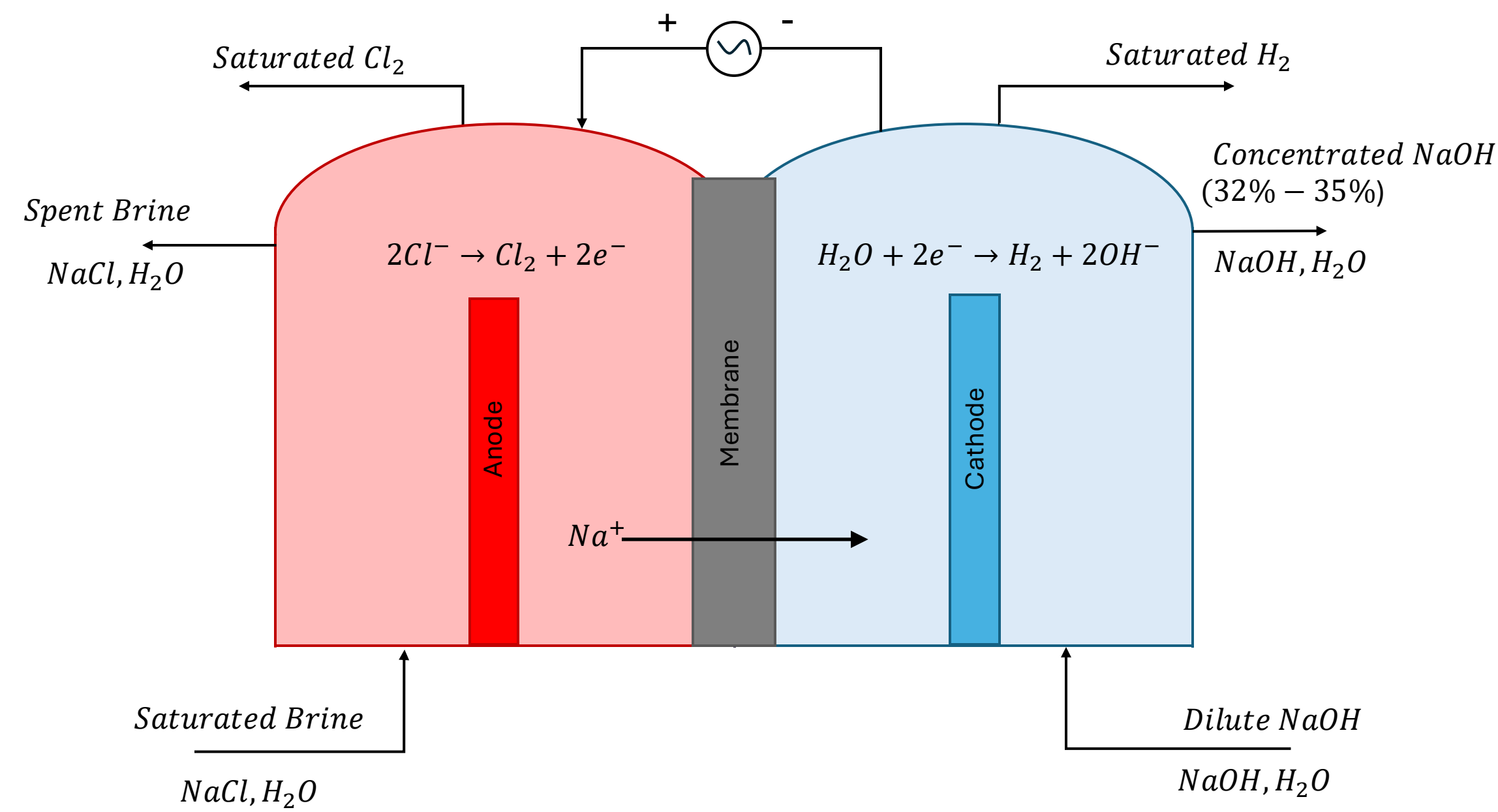
The Baltimore/Maryland region has strong demand for chlorine in water treatment, pharmaceuticals, and manufacturing, yet it currently relies on long-distance transport due to the lack of local production. Developing a local, membrane-based plant improves supply reliability, reduces transportation risks, and enhances overall process efficiency through byproduct integration.



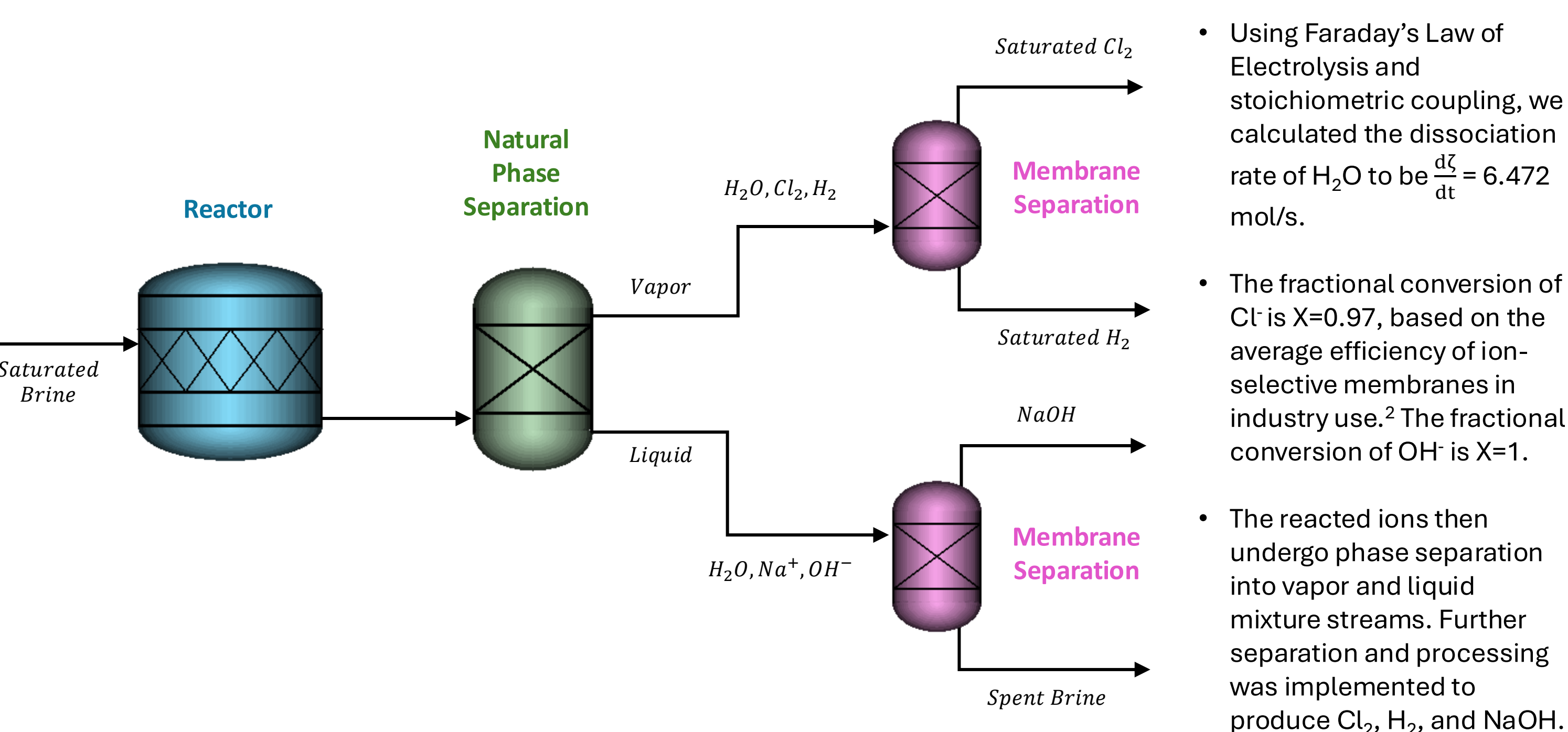
Common applications of chlorine across household, industrial, and public health sectors<sup>1</sup>

## Membrane Electrolysis Modelling

- A sheet of ion-selective membrane allows unidirectional transfer of sodium ions and water molecules.
- Sodium chloride dissociates into sodium and chloride ions in the anode compartment. The chloride ions are oxidized to produce chlorine gas.
- Water in the cathode compartment is reduced to hydrogen gas and hydroxyl ions. Sodium ions combine with hydroxyl ions to form caustic soda.



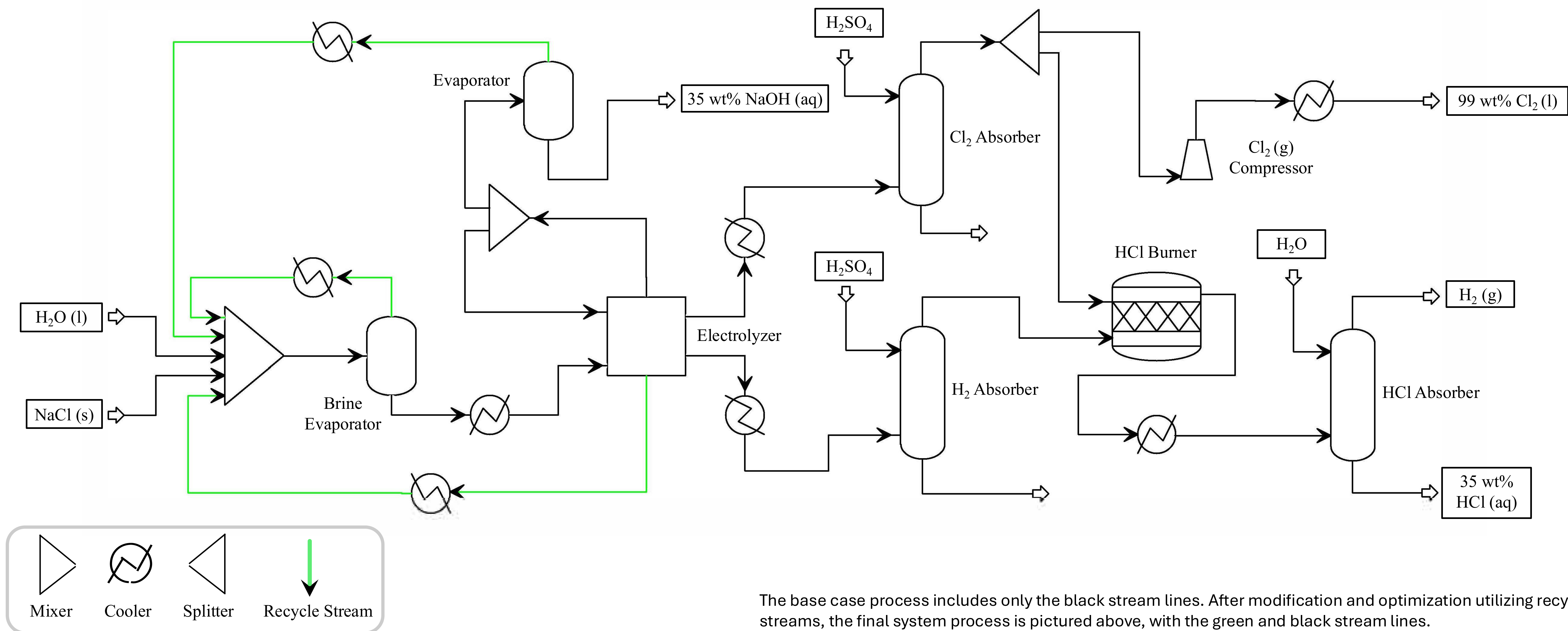
Design of pseudo-electrolysis system, mimicking a membrane electrolytic cell, to isolate desired Cl<sub>2</sub>, H<sub>2</sub>, and NaOH:



- Using Faraday's Law of Electrolysis and stoichiometric coupling, we calculated the dissociation rate of H<sub>2</sub>O to be  $\frac{dX}{dt} = 6.472$  mol/s.
- The fractional conversion of Cl<sup>-</sup> is X=0.97, based on the average efficiency of ion-selective membranes in industry use.<sup>2</sup> The fractional conversion of OH<sup>-</sup> is X=1.
- The reacted ions then undergo phase separation into vapor and liquid mixture streams. Further separation and processing was implemented to produce Cl<sub>2</sub>, H<sub>2</sub>, and NaOH.

## Functional Block Diagram

Process modelling and simulation performed using Aspen Plus®



The base case process includes only the black stream lines. After modification and optimization utilizing recycle streams, the final system process is pictured above, with the green and black stream lines.

## Process Performance & Product Outputs

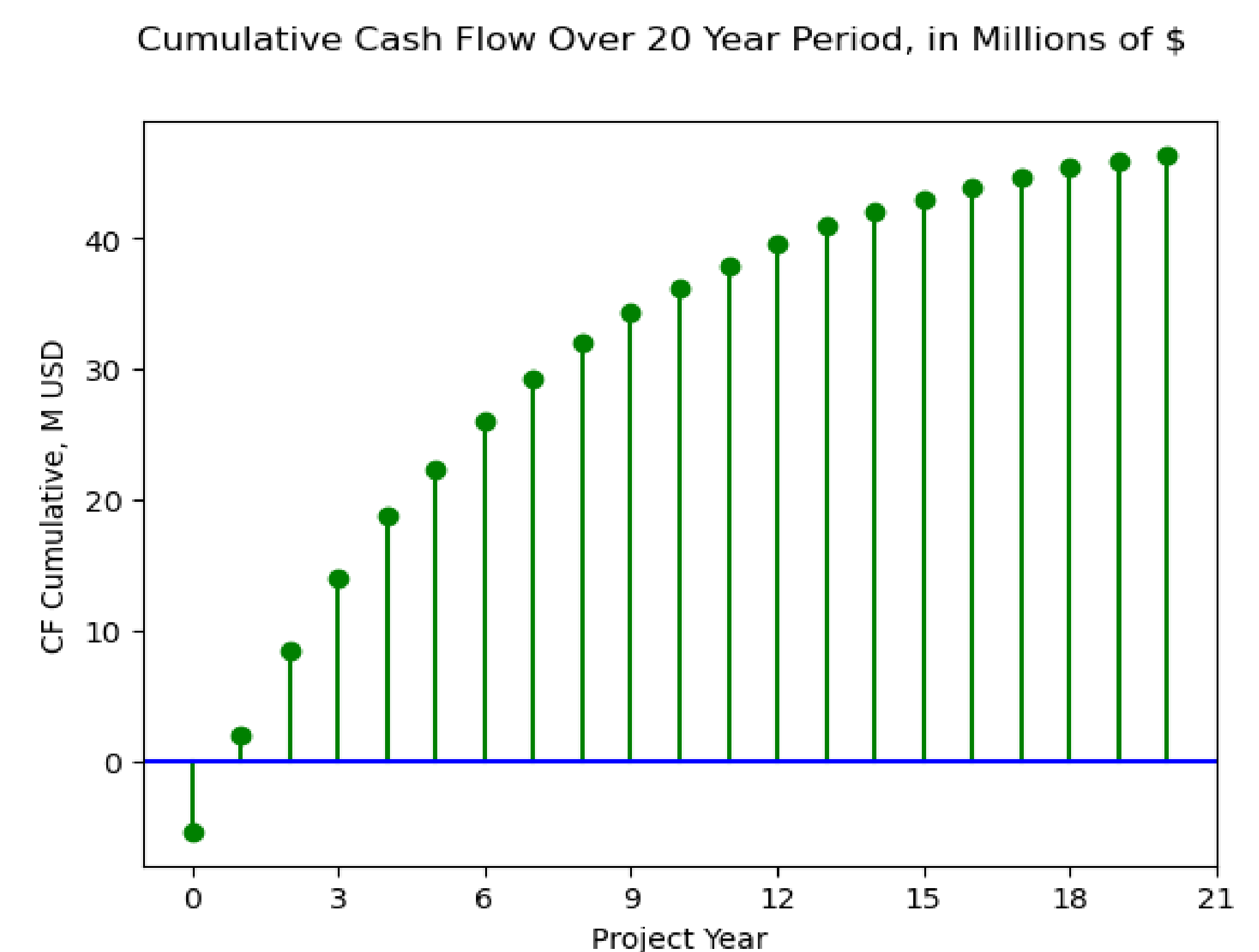
Power Input	Power Output	$\eta$ (% efficiency)
7,673 kW	-1,560 kW	20.33

	Output (tons/day)	% Purity	SEC (kW/ton)
Cl <sub>2</sub>	25.03	99.51	306.56
HCl	51.87	35.04	150.04
NaOH	98.61	50.00	77.81

To optimize performance, recycle streams were implemented in the beginning of the process to reduce the amount of water wasted. Energy produced by the new coolers would be used in a new heat exchanger network (HEN), reducing the overall energy load. The results of these changes can be seen in the table below.

	Modified Results	
Modification	Base Case	Optimized Recycle Modifications
Feed Water Input (tons/day)	232.74	188.03
Power Usage (kW)	7,673	6,113
HEN Power Optimization (kW)	7,673	5,951

## Economic & Sustainability Analysis



$$ROI = \frac{\text{Annual Net Earnings}}{\text{Capital Investment}} = 168.7\%$$

$$RIR = \frac{\text{Water Recycled}}{\text{Water Input}} = 1.49 \quad CCR = \frac{\text{CO}_2 \text{ Fuel Output}}{\text{Cl}_2 \text{ Product}} = 0.43$$

## References

- <https://www.benadryl.com/>, <https://www.clorox.com/>, [https://envremedies.com/envremblog](https://vietnamsteel.com/pvc-https://envremedies.com/envremblog)
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