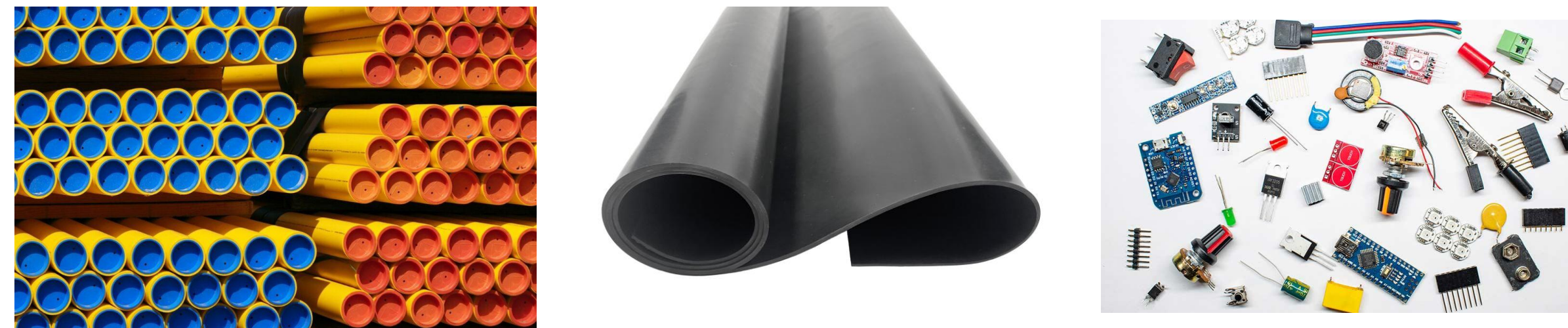


## Introduction & Goals

### Introduction:

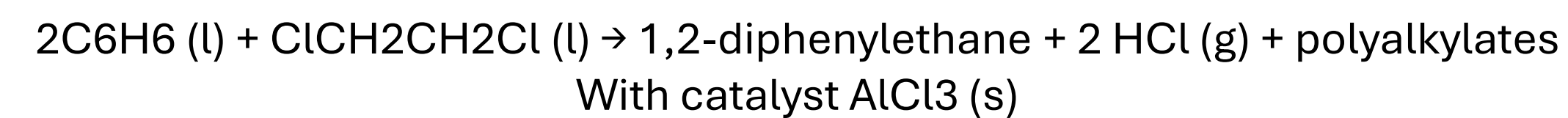
- DPE is a raw material in the production of DBDPE, a brominated flame retardant
- Applications of DPE include use in the textiles, plastics, and electronic industries
- By producing DPE themselves, Albemarle will have control over the amount and purity of DPE
- Additionally, DPE production is profitable as determined by a due diligence analysis



### Goals:

- Design a chemical plant to produce 5000 metric tons of 1,2-diphenylethane (DPE) with a minimum purity of 99 wt% annually
- Develop a PFD, simulate an ASPEN model, and create equipment and stream tables
- Produce a cost analysis within +/- 50%, cumulative cash flow, and operating costs
- Assess potential process hazards (HAZOP) and sustainability impact

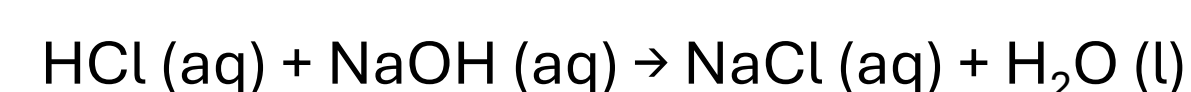
## Technical Background



- The main reaction for DPE above includes an excess of benzene and aluminum chloride catalyst
- The reactor must be maintained at a constant temperature despite the reaction being exothermic
- A heating jacket, filled with steam, makes sure the reactor stays above the boiling point of benzene



- The above reaction is the catalyst deactivation, which is required for stopping the reaction
- The by-product hydrochloric acid warrants major safety concerns, so this reaction will need to be constantly monitored
- Some ways to mitigate the reaction include storing aluminum chloride in a dry environment and implementing moisture control during the reaction



- The above reaction is used to neutralize the hydrochloric acid and utilizes aqueous caustic soda
- This reaction is exothermic but excess water ensures the reaction is maintained at a constant temperature
- As the reaction settles, the mixture is separated between an aqueous and organic phase based on density

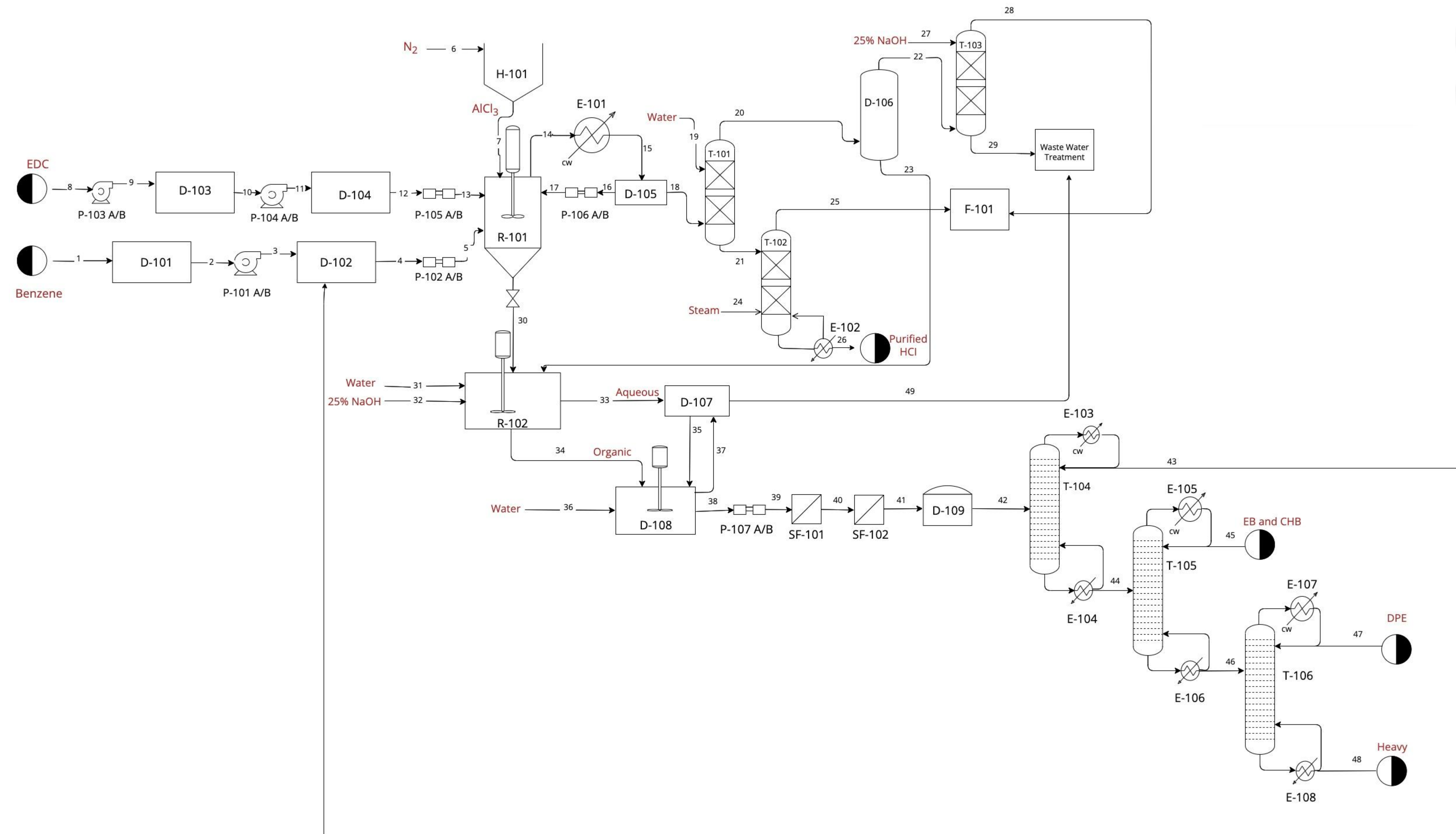
## Safety

- A Hazard and Operability study (HAZOP) analysis was completed to assess process safety and possible hazards
  - Major process hazards include chemical compatibility, HCl corrosion, and temperature/pressure conditions
- A chemical compatibility study showed incompatibilities between EDC and the catalyst, HCl and NaOH, and EDC and HCl
- Although benzene and aluminum chloride catalyst are necessary in the production of DPE, this reaction requires attention as it generates significant heat
- Mitigative Actions:
  - Constant monitoring of controls systems
  - Routine cleaning of equipment
  - Routine equipment inspections
  - Redundant ventilation systems
  - Flow and valve control

## References



## Process Flow Diagram



## Distillation Train Simulation Results

Stream Name	42	43	44	45	46	47	48
Temperature (F)	77.00	176.3	353.5	208.6	592.8	536.9	684.0
Pressure (psia)	30.00	14.70	29.39	14.70	44.09	14.70	56.20
Vapor Mass Fraction	0	0	0	0	0	0	0
Mass Flow (lb/hr)	11020	8591	2431.8	256.3	2176	1482	693.6
Component Mass Fraction							
DPE	0.1578	2.38E-37	0.7151	0.1787	0.7783	0.9895	0.3273
Benzene	0.7893	1	0.0449	0.4265	2.26E-08	3.31E-08	0
CHB	0.0006	1.57E-31	0.0026	0.0218	0.0004	0.0005	1.67E-15
EB	0.0087	4.96E-10	0.0392	0.3721	6.87E-07	1.01E-06	5.53E-34
Heavy	0.0437	5.61E-35	0.1981	0.0009	0.2213	0.0099	0.6727

- DPE product leaves T-106 at 99 wt% and with a flowrate of 1482 lb/hr
  - With an 85% overall equipment effectiveness this produces 15,000,000 lbs a year
- D-109 is a storage tank that stores multiple batches and separates the batch process from the continuous running distillation train
- Pure benzene is stripped in T-104 and recycled back to D-102, to prevent side reactions from occurring in R-101
- All distillation columns use sieve trays

## Cost Analysis

Equipment	Cost
Heat Exchangers	\$244,800
Reactors	\$396,768
Towers	\$316,730
Vessels	\$693,890

- Cost of Manufacturing (COM) was calculated by utilizing cost of labor, utilities, raw materials, waste treatment, and the fixed capital investment
  - Majority of our cost stems from raw materials due to the annual amount of DPE produced
  - COM helped visualize cash flow analysis to illustrate this process does not retain a profit due to it being a precursor for DBDPE

- Major pieces of equipment were inputted into CAPCOST
  - CAPCOST utilized material of construction and sizing of equipment
- Equipment cost represents fixed capital cost
  - Used the summation of cost of equipment to aid in calculation of COM

COM <sub>d</sub> = 0.18FCI + 2.73C <sub>OL</sub> + 1.23(C <sub>UT</sub> + C <sub>WT</sub> + C <sub>RM</sub> )	
Fixed Capital Investment (FCI)	\$1,652,188
Cost of Labor (C <sub>OL</sub> )	\$648,900
Cost of Utilities (C <sub>UT</sub> )	\$700,664
Cost of Waste Treatment (C <sub>WT</sub> )	\$360,160
Cost of Raw Materials (C <sub>RM</sub> )	\$14,108,366
<b>Cost of Manufacturing (COM<sub>d</sub>)</b>	<b>\$20,726,997</b>