

Process Development for the Production of Acetic Acid from Acetaldehyde

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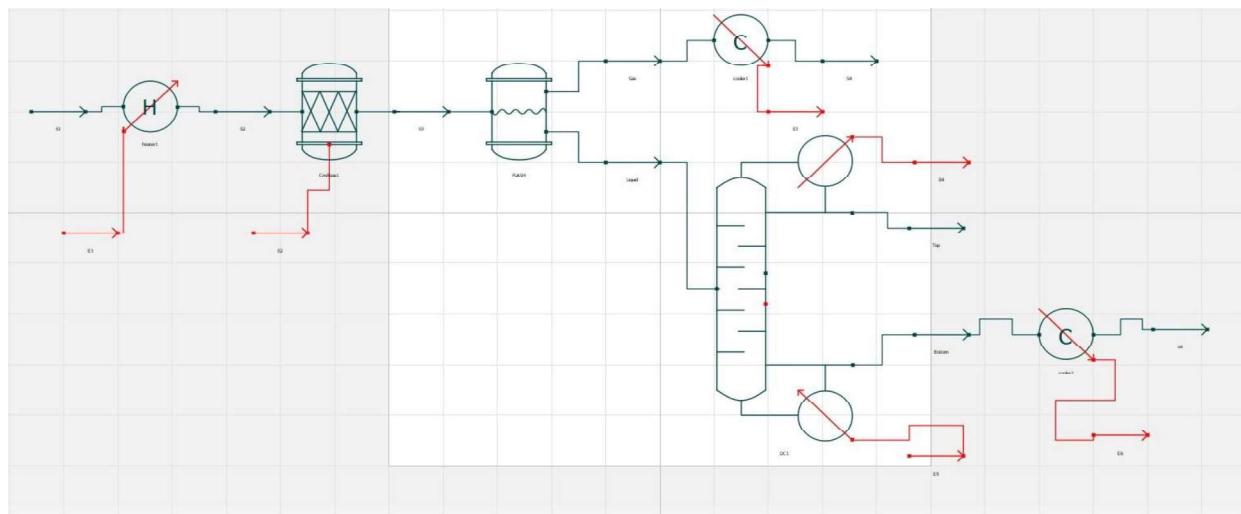
A. Background

Acetic acid, also called as Ethanoic acid, is a colorless liquid organic compound with the molecular formula CH_3COOH . When undiluted, it is called glacial acetic acid. Vinegar is roughly 3–9% acetic acid by volume, making acetic acid the main component of vinegar apart from water. Acetic acid has a distinctive sour taste and pungent smell. It is mainly produced as a precursor to polyvinyl acetate and cellulose acetate. It is classified as a weak acid as it partially dissociates in solution, however concentrated acetic acid is corrosive and can damage the skin. The global demand for acetic acid is about 6.5 million metric tons per year (Mt/yr), of which approximately 1.5 Mt/yr is met by recycling and the remainder is manufactured from methanol.

B. Description of Flow Sheet

This flow sheet was adapted from Shreve (1956) [2]. The feed was first pre-heated to a temperature of 338.15 K at atmospheric pressure. Then the pre-heated feed was fed to a conversion reactor where the conversion was assumed to be 75% with respect to acetaldehyde. The product stream was then sent to a flash column where acetic acid and oxygen get separated, i.e. oxygen at top and acetic acid at bottom. The top product was sent to cooler for cooling to room temperature while the bottom product i.e. acetic acid was sent again to Distillation Column for further purification where acetic acid was purely obtained from bottom product. After that this bottom product was cooled to room temperature.

C. Flowsheet



D. Results

The process flow sheet was simulated for a typical capacity of acetic acid at a temperature of 338.15 K and at atmospheric pressure. Conversion of 75% of Acetaldehyde was assumed in the “conversion reactor” in OpenModelica. A flash column was simulated to separate the gaseous and liquid product. After separating liquid and gaseous product cooler was used to cool the product upto room temperature.

Class A Results						
Object	S1	S4	S5	Flash Gas	D-1 Bottom	Units
Temperature	298.15	298.15	298.15	338.15	316.945	K
Pressure	101325	101325	101325	101325	101325	Pa
Molar Fraction (Mixture) / Acetaldehyde	0.5	0.219218	0.0449	0.219218	0.00377	
Molar Fraction (Mixture) / Oxygen	0.5	0.64166	0.000006	0.64166	0.00234	
Molar Fraction (Mixture) / Acetic acid	0	0.139122	0.943895	0.139122	0.99	

D. Conclusion and Remarks

This study shows that open source process simulator can be used for simulating process and development of process flow sheets. This work can be extended to simulate production of acetic acid from Ethanol. Further, in the present work, the unreacted acetaldehyde and oxygen can be recycled to increase the yield of acetic acid. This study also shows that open source simulators can be used as an effective learning tool to simulate different scenarios like energy stream integration and study their effect.

E. References

1. https://en.wikipedia.org/wiki/Acetic_acid
2. Shreve R. N., The Chemical Process Industries, 2nd Edition, Mc Graw Hill, 1956, p 690