Process Development for the Production of 30 TPD 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 [1].

B. Description of Flow Sheet

This flow sheet was adapted from Shreve (1956) [2].

The feed was first pre-heated to a temperature of 65°C 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 distillation column where acetaldehyde and oxygen were obtained as distillate stream and acetic acid as bottoms. The product stream was then brought to room temperature.

C. Results

The process flow sheet was simulated for a typical capacity of 30 TPD of acetic acid at a temperature of 65°C and at atmospheric pressure. Conversion of 75% of Acetaldehyde was assumed in the "conversion reactor" in DWSIM. A shortcut distillation column was simulated to calculate the actual number of stages, minimum number of stages, location of feed stage and minimum reflux ratio for the given light key and heavy key compositions. In the shortcut distillation column, acetaldehyde was taken as the light key component and acetic acid as the heavy key component. The light key composition at the bottoms was fixed at 0.01 and the heavy key composition in the distillate was fixed at 0.01 and a reflux ratio of 7 was assumed for the shortcut column. The shortcut column was simulated and a minimum reflux ratio of 0.18 was obtained with actual number of stages equal to 3. The amount of energy released per kg of acetic acid produced as a result of this process equals to 4837.62 kJ.

In the next flow sheet (Case B), acetic acid was produced but with the integration of energy streams. In this case, the amount of energy released per kg of acetic acid produced equals to 4703.09 kJ.

In the both the cases (Case A and Case B), the results obtained from the respective shortcut distillation columns were used to specify the input parameters for the simulation of complex columns using CAPE-OPEN Unit Operation. In both the complex columns, the same input specifications (reflux ratio of 0.186 and mole faction of Acetic Acid in the bottoms equal to 0.99) were assumed.

A product flow rate of 1255.10 kg/h was obtained which corresponds to 30 TPD of acetic acid.

Case A Results				
Object	S-1A	S-7A	S-8A	
Temperature	25	38.698187	25	C
Pressure	1.01325	1.01325	1.01325	bar
Mass Flow	2200	944.90465	1255.0954	kg/h
Molar Flow	57.855456	26.051513	20.955628	kmol/h
Molar Fraction (Mixture) / Acetaldehyde	0.5	0.26955485	0.0099999999	
Molar Fraction (Mixture) / Oxygen	0.5	0.69399691	9.9888109E-11	
Molar Fraction (Mixture) / Acetic acid	0	0.036448239	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.

Unit System: (Custom 5 in DWSIM)

Temperature - °C

Pressure - bar

Molar Flow Rate – kmol/h

Mass Flow Rate – kg/h

Volumetric Flow Rate – m3/h

Density – kg/m3

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