A HYSYS Simulation Project for the Production of Synthetic Ethanol by Hydration of Ethylene

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Abstract: Ethanol is very commonly used as a feedstock in the chemical industries. It is also used as fuel and as a solvent. The catalysts are used and widely studied in this field. Nowadays, Ethanol is produced both as a petrochemical, through the hydration of ethylene and, via biological processes, by fermenting sugars with yeast. But production of synthetic ethanol is mainly done through the hydration of ethylene. This process of synthetic ethanol production is simulated using HYSYS simulation software. The purpose of this simulation was to observe the thermodynamic properties of the process and the heat consumption. Also it was useful to understand the changes that will occur if properties of each unit were changed. Though the simulation showed a slight deviation from the literature value, it was helpful to understand the process along with other thermodynamic properties. Since pilot plants are expensive for this type of case, HYSYS gives us an opportunity to observe and realize the plant and the process happening inside.

Keyword: Synthetic ethanol, Ethylene, HYSYS.

I. INTRODUCTION

Ethanol as one of the most well-known oxygen-containing organic materials has a wide variety of applications. Ethanol in medical applications such as sterilization of medical instruments, dressings, directly in the formulation of some drugs and nonmedical costs, as additives to fuel motor vehicles, production of vinegar, a variety of solvents, paints and other fields of application are numerous (Renewable Fuels Association, 2012). Official statistics illustrate that global produced ethanol was around 1.02 10¹¹ liters in year 2010 (Ethanol Industry News, 2011). Most ethanol (approximately 93 percent) in the world is produced through fermentation and only about 7 percent is made synthetically (Nelson, 1951; Maki et al, 1998). The principal suppliers of synthetic ethanol are multi-national companies’ plants like Sasol companies in Europe and South Africa, Equistar Company in the United States and SADAF Company in Saudi Arabia (Ethanol Industry News, 2011). The initial stages and materials vary based on production methods of ethanol. Moreover, the biggest synthetic ethanol manufacturing plants are in Germany and Scotland with a production rate of 1.7 10⁸ liters per year (Gilmartin, 2005; Bristow, 2011).

It has been declared that ethanol production through fermentation is much too volatile to allow for a secure and constant supply of ethanol in the region (Chemical Industry News & Intelligence, 1998). On the other hand, it is said that synthetic production of ethanol seems to be less economical in the U.S. which is due to high costs of ethylene, the initial materials of the Regarding the existence of many incomplete and unoptimized technologies for the production of reaction, and the great features of their farming products that allow them use fermenting methods for agricultural wastes (Chemical Industry News & Intelligence, 1998, 2005). Figure 1 shows the main global exports of ethanol in 2005 (FO Licht, 2006).

Economic estimation of ethanol production conditions differs based on geographical locations; In the U.S. for instance, synthetic method of ethanol production tends to decrease while in a country like Saudi Arabia, having similar features to Iran and other Middle East countries, it is considerably increasing (Logsdon, 1994; SADAF, 2010). In the region of Middle East, countries like Saudi...
Arabia And Qatar are using this production method in some companies; however, it has not yet been widely used and spread (Gilmartin, 2005; Logsdon, 1994).

In the current decade, due to focusing on environmental concerns and environmental friendly technologies, bioethanol has become a valuable and strong option in the global energy market as an additive for vehicles. Consequently, the development of cost-effective technologies for fuel ethanol production has been a priority for many researchers and also governments. Ethanol process engineering tools and functions are highly required. Process engineering applied to the production of fuel ethanol includes the design of new innovative process configurations which implies reducing fuel ethanol production costs. After all, design process of synthesis, makes a good opportunity for the formulation of finding the most improved technoeconomic and environmental industry (Carlos & Oscar, 2007). As a result, process optimization is another vital element that must be utilized in the framework of the process.

II. BRIEF HISTORY OF PROCESS

Ethanol was first prepared synthetically in 1825 by Michael Faraday. He found that sulfuric acid could absorb large volumes of coal gas. He gave the resulting solution to Henry Hennell, a British chemist, who found in 1826 that it contained “sulphoyinic acid” (ethyl hydrogen sulfate). In 1828, Hennell and the French chemist GeorgesSimon Sérullas independently discovered that sulphovinic acid could be decomposed into ethanol. Thus, in 1825 Faraday had unwittingly discovered that ethanol could be produced from ethylene (a component of coal gas) by acid-catalyzed hydration, a process similar to current industrial ethanol synthesis.

Ethanol was used as lamp fuel in the United States as early as 1840, but a tax levied on industrial alcohol during the Civil War made this use uneconomical. The tax was repealed in 1906. Original Ford Model T automobiles ran on ethanol until 1908. With the advent of Prohibition in 1920, ethanol fuel sellers were accused of being allied with moonshiners, and ethanol fuel fell into disuse until late in the 20th century.

In modern times, ethanol intended for industrial use is also produced from ethylene. Government interference in the market place and the demand for production from the huge surplus of grain has not changed the economics: alcohol from ethylene is purer and cheaper. Ethanol has widespread use as a solvent of substances intended for human contact or consumption, including scents, flavourings, colourings and medicines. In chemistry, it is both an essential solvent and a feedstock for the synthesis of other products. It has a long history as a fuel for heat and light, and more recently as a fuel for internal combustion engines.

III. PROCESS DESCRIPTION

Ethylene and water were fed to the mixer and well mixed gas at feed pressure and 21°C was fed to the heater for being heated up to 100°C Celsius. Then the heated mixture was available for reaction in reactor-1 where 60% of the fed ethylene was converted into ethanol, in this reaction.
phosphoric acid was used as catalyst. The rest ethylene was converted into acetaldehyde in reactor-2. The vapour phase effluent was then entered into separator and then into reactor-3 where the available acetaldehyde was converted into ethanol by added hydrogen. Effluent gas from reactor was then cooled down to 15° Celsius by cooler. The cooled gas was then fed into separator where we got both liquid and gas phase effluent. The liquid phase effluent was fed into distillation column after being heated up to 400° Celsius by heater-2. From distillation column we get the desired product and residue.

IV. REACTIONS

The reactions in the process are as follows:

\[ \text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{CH}_2\text{OH} \]

\[ \text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2 \]

\[ \text{CH}_3\text{CHO} + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{OH} \]

V. SIMULATION OF THE PROCESS

In this modern age of powerful computers, it often makes no sense to put pencil to paper like in the old days. Now, new software can perform repetitive chemical engineering calculations in a fraction of the time it takes to execute them by hand. Process simulation is used for the design, development, analysis, and optimization of technical processes and is mainly applied to chemical plants and chemical processes, but also to power stations, and similar technical facilities. Process simulation is a model-based representation of chemical, physical, biological, and other technical processes and unit operations in software. Basic prerequisites are a thorough knowledge of chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models which, in combination, allow the calculation of a process in computers.
Process simulation software describes processes in flow diagrams where unit operations are positioned and connected by product streams. The software has to solve the mass and energy balance to find a stable operating point. The goal of a process simulation is to find optimal conditions for an examined process. This is essentially an optimization problem which has to be solved in an iterative process.

Process simulation always uses models which introduce approximations and assumptions but allow the description of a property over a wide range of temperatures and pressures which might not be covered by real data. Models also allow interpolation and extrapolation - within certain limits - and enable the search for conditions outside the range of known properties.

So the benefits of Process Simulation Modelling can be stated as-

- Creating a process simulation model can provide several benefits for new and existing processes. The ability to simulate process behavior without the costs of pilot trials or test runs can save man-hours and lost production, in addition to avoiding safety concerns that might arise when changing operational specifications.

- Visualizes effects of process changes-
  - Simulate changes to see mass/energy balance effects within a plant
  - Especially beneficial for plants with heat integration and recycled process streams
  - Locate bottlenecks and determine new process limitations if bottlenecks are removed
  - Simulate effects of equipment modifications for heat exchangers, distillation columns, scrubbers, reactors and more.

- Track and minimize utility consumption -
  - See where heating a cooling streams energy is going, and how to minimize it
  - Compare simulation utility consumption to process data to find energy leaks and inefficiencies.

- Gives insight to process controls and operations -
  - Helps understand relationships between controlled and manipulated process variables
  - Establish control set points for various production scenarios by optimizing process centerlines.

5.1 Brief Unit Description

Following units are involved in our simulation-

- Mixer
- Heater
- Converter reactor
- Separator
- Cooler
- Distillation column

They are described shortly in below-
5.1.1 Mixer

Mixes two or more fluid stream input and gives one output.

5.1.2 Heater

This unit heats up the feed to desired temperature by specifying the pressure drop and outlet Pressure.

5.1.3 Converter reactor

It is an equilibrium Reactor chosen from the library. It is used for the equilibrium reaction sets only. This reactor is valid both for exothermic and endothermic reactions. It is also possible to maintain a constant temperature in the reactor by removing or supplying heat.

5.1.4 Separator

It is used for separating liquid and vapor mixture in given process stream at a constant temperature or by inputting or removing heat. It is also possible to add reaction sets here.

5.1.5 Cooler

It is used to cool the process stream to desired temperature.

5.1.6 Distillation column

It is the most versatile tool in HYSYS. Any kind of distillation is possible in this unit. It works by separating most volatile components from a process feed.

**Figure 03: Simulation of the process**

### VI. RESULT AND DISCUSSIONS

**Table 01: Table showing the result of the simulation**

<table>
<thead>
<tr>
<th>Product Stream</th>
<th>Flow Rate, (Kmol/hr)</th>
<th>Ethanol Present, (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Product</td>
<td>750</td>
<td>64.97</td>
</tr>
</tbody>
</table>
In Case study 1, graph for composition for ethanol in product stream vs. distillation in temperature is plotted. From the graph, we see composition of ethanol in product decreases rapidly with temperature increase in distillation column up to a range and then becomes almost constant.

![Graph for ethanol composition in product stream vs. distillation in temperature (°C)](image)

**Figure 04:** Graph for ethanol composition in product stream vs. Distillation in Temperature (°C)

In Case study-2, relation between compositions of ethanol in product with feed temperature is shown. As we see from the graph, the feed temperature has no effect on product composition.

![Graph for change of composition of ethanol in product with feed temperature (°C)](image)

**Figure 05:** Graph for change of composition of ethanol in product with feed temperature (°C)

In Case study-3, relation between product molar enthalpy with temperature of distillation in stream is shown. As we see from the graph, the product molar enthalpy decreases linearly with the increase in temperature of the ‘distillation in’ stream.
VII. CONCLUSION

Synthetic ethanol production is a very well-known chemical process that is widely used for large range ethanol production. In our paper, we have generated data based on the simulation performed in HYSYS. We did simulation for a very simplified process. Additional unit operations blocks can be used to optimize production or maximum profit. As this is a simplified model, so this model will be very much helpful understanding the process and the economics, and also is a starting point for more sophisticated models for plant designing and process equipment specifying.

REFERENCES


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