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Simulation of ethylene oxide production from ethylene cholorhydrin

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Summary. This research has been performed in the Ethylene Oxide production process. It is a flammable and colorless gas at temperatures above 11 °C. It is an important commodity chemical for the production of solvents, antifreeze, textiles, detergents, adhesives, polyurethane foam, and pharmaceuticals. Small amounts of Ethylene Oxide [EO] are used in manufacturing fumigants and sterilants for spices and cosmetics, as well as hospital sterilization for surgical equipment. Modern Ethylene oxide [EO] productions employ either air or oxygen (O_2)to oxidize ethylene (C_2H_4) with a silver catalyst on an alumina oxide carrier[Ag/Al_2O_3]catalyst packed in a fixed-bed reactor (plug-flow reactor)but the oxygen-base reaction process is more desirable here we used oxygen. Mainly two reactions occur, partial oxidation of ethylene to ethylene oxide and total oxidation of ethylene to carbon dioxide and water. The design models of the process in this research based on a three-part system. They are: the reaction system, absorption system and Ethylene Oxide [EO] purification system. The largest cost in production of ethylene oxide is ethylene therefore, it's important to optimize the selectivity towards ethylene oxide and thus reduce the consumption of Ethylene. The aim of this work is to create a simulation model of the Ethylene Oxide production process from Ethylene using Aspen Hysys V9. Also to knowing the optimum operational conditions (temperature –pressure –flow rate) for the oxidation reactions of Ethylene. The simulation was running three times with various operational conditions to make a good result. The conclusion was that during operational time the activation energy increased for both reactions which have to be compensated with increasing reactor temperature. At the same time the selectivity for producing Ethylene Oxide decreases, i.e. more carbon dioxide and water are formed. The simulation models yield Ethylene Oxide with purity of 99.2%.

Keywords: simulation, municipal solid, gasification, fixed bed reactor, pyrolysis, gibbs energy, rgibbs model, gasifier

Introduction

Ethylene: Ethylene is widely used in chemical industry, and its worldwide production (over 109 million ton in 2006) exceeds that of any other organic compound. It mostly used to produce three chemical compounds: Ethylene Oxide, Ethylene dichloride, Ethyl benzene, and a variety kinds of Polyethylene. Moreover, it is an ideal base material for many other petrochemicals, as it is readily available at high purity, low cost, and usually reacts with other low cost components, such as Oxygen and water. Currently, Ethylene is produced in the petrochemical industry by thermal cracking of a lkanes such as Ethane, Propane, Butane, Naphtha and gas oil. The choice of feedstock is an important economic issue as it influences other costs as well. In this process, feed stocks are heated to 700 – 900oC. This process converts large hydrocarbons into smaller ones and introduces un saturation. The reactor effluent is quickly quenched to avoid further reaction, then compressed, and finally sent to a separation unit for the recovery of Ethylene and other products such as Methane, Ethane, propane, Propylene, Butylenes, and Pyrolysis gasoline. Ethylene Oxide (EO) is a flammable and colorless gas at temperatures above 11 °C, which smells like ether at toxic levels. It is an important commodity chemical for the production of solvents, antifreeze, textiles, detergents, adhesives, polyurethane foam, and pharmaceuticals. Small amounts of EO are used in manufacturing fumigants and sterilants for spices and cosmetics, as well as hospital sterilization for surgical equipments. Modern EO productions employ either air or Oxygen (O_2) to oxidize Ethylene (C_2H_4) with $Ag/Al_2 O_3$ catalyst packed in a fixed-bed reactor (plug-flow reactor). The Oxygen-based reaction process is more desirable because of four major benefits: (i) higher productivity and selectivity; (II) lower initial capital costs; (III) less expensive catalyst required; and (IV) less air pollutants resulting from the purge gas .Industrial production of Ethylene Oxide:

1. Wurtz-process:
2. Direct oxidation process:

Materials and Methods

Simulation: Simulation is a situation in which a particular set of conditions is created artificially in order to study or experience something that could really exist in reality. It is the act if pretending that something is real when it is not. A computer simulation is an attempt to model a real-life or hypothetical situation on a computer so that it can be studied to see how the system works.

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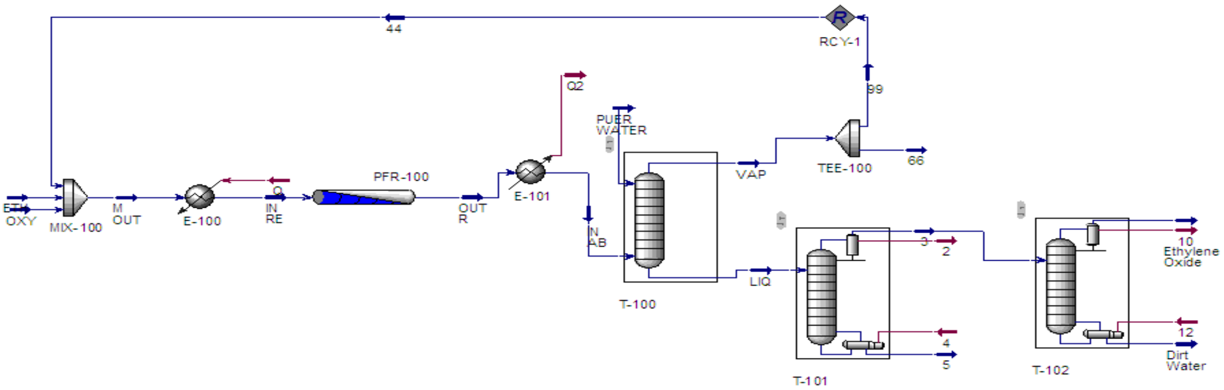

Figure 1.Simulation flow diagram of Ethylene Oxide production

Table 1.

Main shortcut from figure (1)

Name	Object Type	Name	Object Type
MIX-100	Mixer	TEE-100	Tee
E-100	Heater	RCY-1	Recycle
PFR-100	Plug Flow Reactor	T-101	Distillation
E-101	Cooler	T-102	Distillation
T-100	Absorber		

Results and Discussions

The Effect of Operating Condition: In this section, we see the influence of operating condition (temperature, pressure and flow rate) in Ethylene Oxide [EO] production

The Effect of flow Rate: The Effect of Ethylene flow Rate on Ethylene Oxide Production:

Figure (1) shows the Ethylene Oxide molar flow increases with Ethylene molar flow increases.

The Effect of Oxygen Flow Rate on Ethylene Oxide Production: Oxygen flow rate has positive effect in the production of Ethylene Oxide as we show figure (2). The reaction for production Ethylene Oxide is exothermic (shown in figure (3)). The temperature has negative effect in the production of Ethylene Oxide.

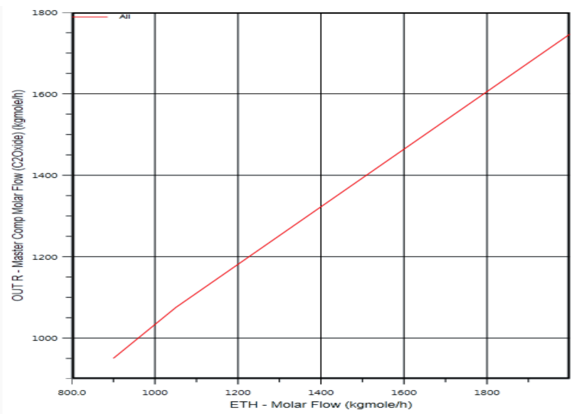

Figure 2. The effect of Ethylene flow rate on Ethylene Oxide production

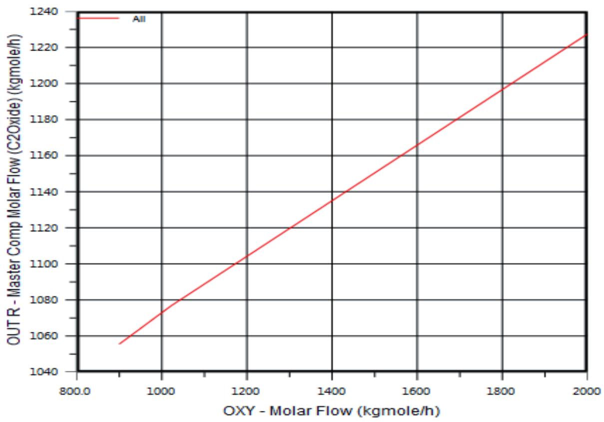

Figure 3. The effect of Oxygen flow rate on Ethylene Oxide production

The Effect of Temperature on Ethylene Oxide production: The reaction between Ethylene and Oxygen has main product (Ethylene oxide) increases when temperature decreases (shown in figure 4) and by product (CO_2&H_2 O) increases with temperature, has high value at 250 °C and decreases above it.

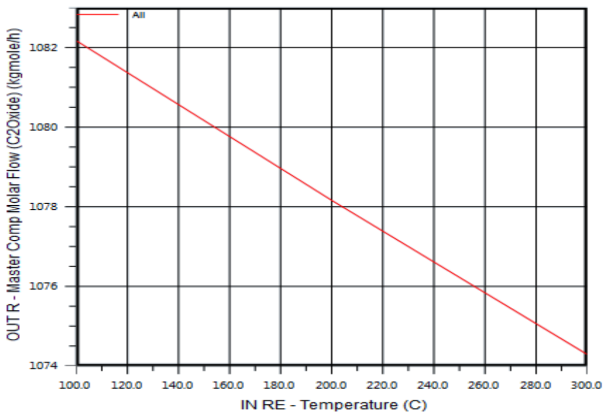

Figure 4. The effect of Temperature on Ethylene Oxide production

The Effect of Pressure on Ethylene Oxide production: Figure (6) shows the pressure has negative effect the flow rate of product decreases with pressure increases. The reaction between Oxygen and Ethylene occurs under a pressure of approximately 2000 kPa and a temperature of approximately 250 °C.

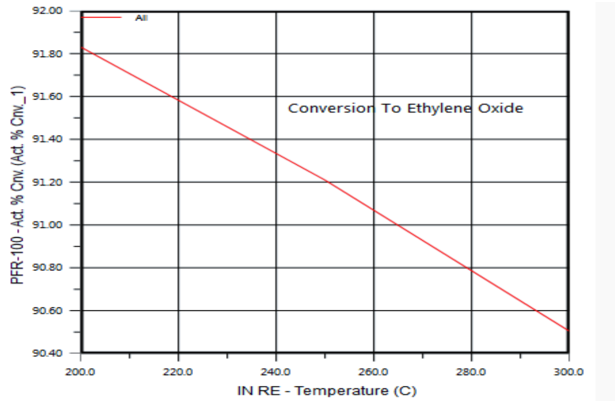

Figure 5. The effect of Temperature on Ethylene partial oxidation

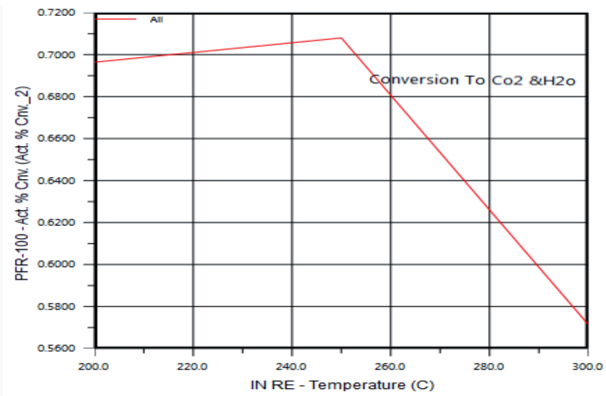

Figure 6. The effect of Temperature on Ethylene total oxidation

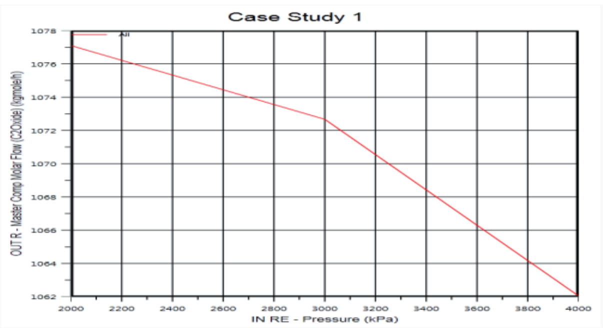

Figure 7. The effect of Pressure on ethylene oxide production

Conclusions

The oxidation process was simulated by the aspen (Hysys) software version.9 and it gave good results for operating condition. One of the most important results obtained from this work is that, it is very important to make analysis for the process operating condition. From this results, it can be seen that the optimum temperature to yield high amount of Ethylene Oxide is 200° C. But It has been proven that, the process was favored at a pressure of approximately 2000 kPa and a temperature of approximately 250 °C over a silver catalyst on an alumina oxide carrier. The results of simulation show that, high amount of Carbon dioxide and water contained at 250 °C. The selectivity towards Ethylene Oxide was decreasing over time and this is a result from deactivation of the catalyst. When this deactivation takes place, more Ethylene is more oxidized form Carbon dioxide and water. The simulation models yield Ethylene Oxide with purity of 99.2 %.

Recommendations

1. Using Aspen HYSYS program to develop any process will be very helpful, because it is very accurate and very helpful in equipment design and selection of the optimum operating conditions.
2. Detail studies must be taken for accurate selection of operation conditions and equipment specifications.
3. The simulation models need further and more study.
4. The simulation models need to add the CO_2 section [CO_2 absorption, CO_2 desorption] in order to: maintain an acceptable CO_2 concentration in the circulated reactor gas, avoid catalyst deactivation and improved selectivity towards Ethylene Oxide production.
5. The stream from the bottom of the second distillation column can be send to the glycol section because it contains Ethylene Oxide and water.

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Contribution

Elrafie A. A. Allah corrected the manuscript, improved the results discussion and put in the format required by the Journal before filing in editing and is responsible for plagiarism editing.

A. Elhameed M.O. Kasif proposed a scheme of the experiments and organized production trials, corrected the manuscript, improved the results discussion and put in the format required by the Journal before filing in editing and is responsible for plagiarism

Yasir A. Mohamed corrected the manuscript, improved the results discussion and put in the format required by the Journal before filing in.

Ayat A. Elkhalig H. Mahmoud review of the literature on the investigated problem, conducted the experiments, performed the characterizations and measurements, and wrote the manuscript

Conflict of interest

The authors declare no conflict of interest.

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