Process Analysis and Optimization of Ethylene Oxide Production

CHE251 (2024-25-I): Term Project Report
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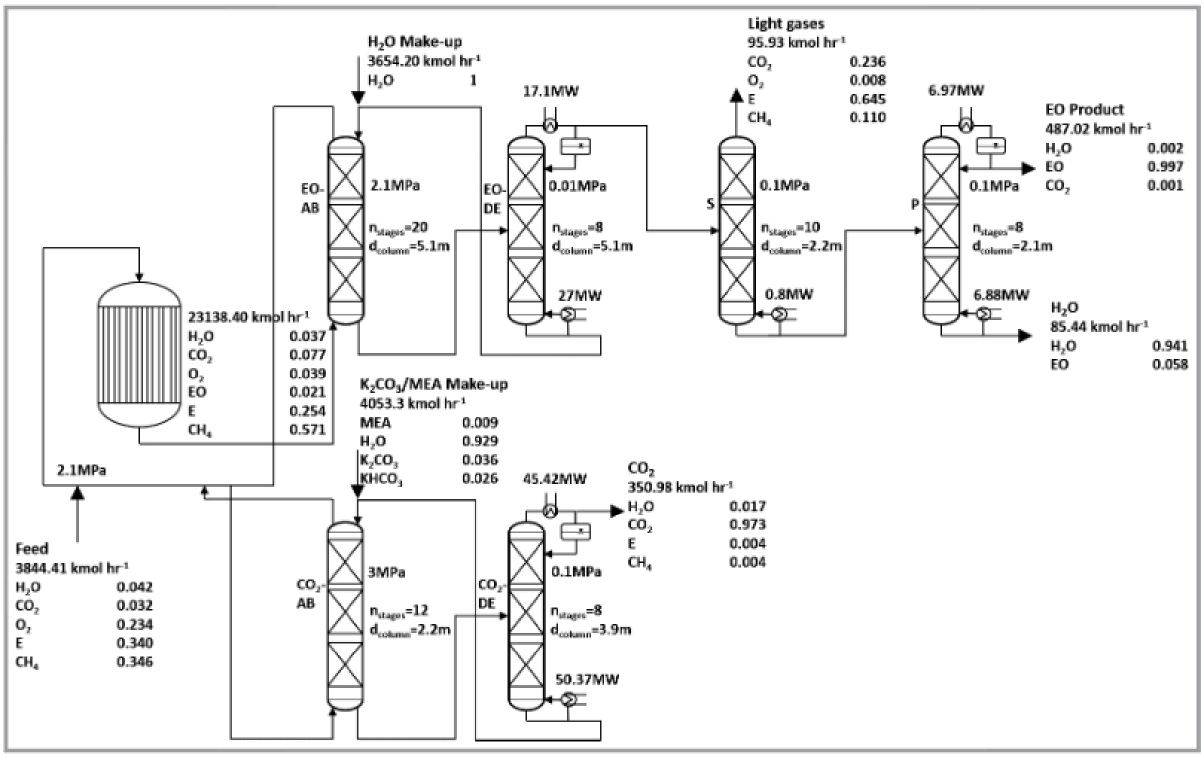

Figure 1: Process Flowsheet

1 Description of the Process

The process focuses on the production of ethylene oxide through the direct oxidation of ethylene using oxygen over a silver-based catalyst in a tubular reactor. The reaction is highly exothermic, requiring efficient cooling achieved by boiling water. The reaction takes place at high pressure (1 to 3 MPa) and moderate temperatures (450 to 545 K), with unreacted reactants recycled through absorption columns to maximize yield and reduce waste.

The process includes:

1. **Reaction**: Ethylene and oxygen are combined in the reactor with a moderator (like nitrogen) to ensure safe operation. The oxidation reaction forms ethylene oxide, along with by-products.

2. **Absorption**: Ethylene oxide is absorbed in water, while unreacted ethylene, oxygen, and by-products are treated and recycled.

3. **Separation and Purification**: Ethylene oxide is separated from water in distillation columns, where further purification occurs to achieve product-grade ethylene oxide.

The reaction for the conversion of ethylene to ethylene oxide typically involves the oxidation of ethylene (C_2H_4) with oxygen (O_2) in the presence of a silver-based catalyst. The process is highly exothermic and occurs at high pressure and moderate temperatures in a tubular reactor. The simplified (not considering any side reactions) chemical reaction for ethylene oxide production is:

$$C_2H_4(g) + \frac{1}{2}O_2(g) \rightarrow C_2H_4O(g)$$

2 Objectives

1. **Analyze the Ethylene Oxide Production Process:** Investigate key unit operations, including the reactor, absorption columns, and distillation columns, to understand their role in the overall process.

2. **Optimize Process Parameters:** Identify areas within the process where optimizations can be made to improve yield, reduce energy consumption, and enhance safety. Also, propose modifications to operating conditions that could lead to a more robust and flexible production process.

3 Methodology

In this ethylene oxide production process, ethylene reacts with oxygen in a tubular reactor, where conditions are carefully controlled to promote ethylene oxide formation while minimizing by-products like CO2. The reaction occurs under high pressure (2.1 MPa) and moderate temperatures, using a silver-based catalyst. Efficient cooling through boiling water ensures the highly exothermic reaction remains safe and manageable.

The feed entering the reactor consists of a mixture of ethylene, oxygen, water, and inert gases like methane. After the reaction, the reactor output, which includes ethylene oxide, unreacted ethylene and oxygen, water, and by-products, is processed through separation and purification units.

Key units include:

- The **Desorber Column**: Separates gas streams, recycling unreacted gases (CO2, O2, and CH4) while capturing ethylene oxide.
- The **Absorption Unit**: Uses water to absorb ethylene oxide, venting or further processing the remaining gases.
- The **Stripper and Refining Columns (Flash)**: Purify ethylene oxide, separating it from water and by-products. Final ethylene oxide is collected, while water and trace gases are recycled or removed.

Our focus is on improving yield, energy efficiency, and resource recycling. Preliminary analysis shows an overall ethylene conversion of approximately 95.15 percent. Relevant molar flow rates and mole fractions are detailed in the flowsheet.

4 Results

Our initial analysis revealed issues with the flowsheet data:

- **Input-Output Discrepancies**: The ethylene oxide output was higher than the amount produced by the reactor.
- **Missing Purge Stream**: The CO2 removal unit lacked a specified purge stream.
- **Unbalanced Streams**: Potassium input in the separator had no corresponding output, indicating the need for a purge stream.
- **Missing column information**: The operating conditions for the distillation/desorption and absorption columns were not completely mentioned in the flowsheet.

To tackle the above mentioned issues we resorted to making 'envelopes' around the different units present in the flowsheet according to our Teaching Assistant's advice. This resulted into formation of 4 different systems around which a material balance was to be performed individually.

As for the simulation of the different columns, we dealt with only the blocks which were part of the course curriculum, that being conversion reactor and flash column.

Component	**Reactor Output**	**H2O Make up**	**Initial Recycle**	**Stream Flash**
(kmol/hr)	23138.4	3654.2	26124.21	668.29
Ethylene	0.252074	0	0.223	0.092
H2O	0.0374184	1	0.169	0.122
O2	0.0381627	0	0.0636	0.001
Methane	0.571739	0	0.506	0.016
CO2	0.0771893	0	0.067	0.035
Ethylene Oxide	0.0234167	0	0	0.734

Table 2: **EO Absorber/Desorber Material Balance** (kmol x/kmol)

Component	**Fresh Feed**	**Main Recycle Stream**	**Reactor Output**
(kmol/hr)	3844.41	19564.9	23138.4
Ethylene	0.34	0.259	0.252
H2O	0.042	0.036	0.0374
O2	0.234	0.013	0.038
Methane	0.352	0.607	0.572
CO2	0.032	0.085	0.077
Ethylene Oxide	0	0	0.0234

Table 1: **Reactor Material Balance** (kmol x/kmol)

Component	**Stream Flash**	**Light gases out**	**Water Out**	**EO Prod**
(kmol/hr)	668.39	95.914	85.298	487.177
Ethylene	0.092	0.64	0	0.0003
O2	0.001	0.0069	0	0
CO2	0.035	0.241	0	0.0005
H2O	0.122	0	0.946	0.0018
Methane	0.016	0.111	0	0
Ethylene Oxide	0.734	0	0.054	0.9975

Table 3: **Flash Material Balance** (kmol x/kmol)

Component	**Initial Recycle**	**MEA**	**CO2 Out**	**Main Recycle**	**Purge**
(kmol/hr)	26124.21	4053.3	350.98	19564.9	11264.68
Ethylene	0.223		0.004	0.259	0.067
H2O	0.169	0.929	0.017	0.036	0.663
O2	0.0636	0	0	0.013	0
Methane	0.506	0	0.006	0.607	0.119
CO2	0.067	0	0.973	0.085	0.125
Ethylene Oxide	0	0	0	0	0
MEA	0	0.009	0	0	0.003
K2CO3	0	0.036	0	0	0.012
KHCO3	0	0.026	0	0	0.009

Table 4: **CO2 Desorber Material Balance** (kmol x/kmol)

The final results of the material balance around the different units are as follows:

- **Reactor:** The reactor has two input streams, a Fresh Feed and a Main recycle stream. (refer Table 1)
  Molar Flow Rate of **Fresh Feed** = 3844 kmol/hr
  Molar Flow Rate of **Main Recycle stream** = 19565 kmol/hr
  Molar Flow Rate of **Reactor Output** = 23138 kmol/hr
  Single Pass Conversion of Ethylene to Ethylene Oxide = 8.5%
  Overall Conversion of Ethylene to Ethylene Oxide = 42.15%
  Yield of Ethylene Oxide = 23.46%

- **First Absorber/Desorber unit*:** This unit comprises of a desorber and absorber column. The input to this envelope is the reactor output stream and a H2O make up stream. There are two outputs, a stream towards the flash distillation columns and another to the CO2 separation unit. (refer table 2)

- **Flash Distillation Columns:** There are two consecutive flash distillation columns with an envelope enclosing both of them. The first Flash column has one input stream coming from the first Absorber/Desorber unit and two output streams being a light gas purge stream and a stream to the next flash column.
  The second flash column has one input and two output streams, one being a water purge stream and the other Ethylene Oxide product stream. (refer table 3)

- **CO2 Separation Unit*:** This unit aims to remove CO2 from the process. It has two inlets, one from the Absorber/Desorber unit and one is a K2CO3 make up stream. Three outlets are there, one is the main recycle stream to the reactor, one CO2 output and the last is the purge stream. (refer table 4)

5 Discussion

The flowsheet was initially analyzed for completeness regarding material balances. We discovered discrepancies and missing information, particularly around recycle and purge streams. After contacting the paper's authors, they confirmed the existence of a purge stream, which was not shown explicitly. This purge stream must be optimized based on the desired results.

We simplified the flowsheet by creating boundaries around multiple units and, after consulting with our Teaching Assistant, are working to restructure the recycle streams. This includes introducing new purge and input streams for individual units to ensure proper material balance.

Further issues included:

- **Missing Purge Stream in CO2 Removal Unit**: Critical for maintaining system balance.

- **Ethylene Oxide Output Discrepancy**: More ethylene oxide was being produced than the reactor should yield, indicating a need for recalibration.

These challenges have hindered our ability to match the flowsheet's results, necessitating optimization efforts.

To address these challenges, we consulted with the Course Instructor and also contacted the original authors of the reference paper. The authors confirmed that a purge stream existed, although it was not explicitly shown in the flowsheet. They advised us to adjust the purge stream values to align with the other specifications in the flowsheet. Following the Instructor's guidance, we created envelopes around the various process blocks to perform material balances. However, due to the lack of complete data regarding the purge stream, we were unable to conduct a thorough energy balance.

To address the issues mentioned, we followed the advice of our Teaching Assistant and created "envelopes" around the various units in the flowsheet. This approach led to the formation of four distinct systems, each of which was analyzed separately using material balances.

*For the simulation of the process, we focused on the units covered in the course curriculum, specifically the conversion reactor and the flash column.

6 Conclusion

In this project, we focused on analyzing and optimizing the ethylene oxide production process, identifying key issues such as discrepancies in material balances, missing purge streams, and unbalanced flows in the system. While these challenges prevented us from finalizing the material and energy balances, significant progress was made in understanding the process flow and pinpointing areas that require further refinement. Through consultation with the course instructor and the original authors of the reference paper, we confirmed the existence of a missing purge stream, which is critical for resolving the identified imbalances.

One of the key achievements of this project was the successful reproduction of the output streams in ASPEN with 98% accuracy, based on the inlet streams calculated manually using material balance techniques. This demonstrates the validity of our calculations and material balance approach. The accurate replication of these output streams confirms the correctness of the process model and serves as a strong basis for future optimizations and further refinement of the ethylene oxide production process.

Some of the ways in which this could be achieved by:

- **Optimize Temperature and Pressure:** EO production typically operates at 200-300°C and 10-30 bar. Fine-tuning these conditions to the most efficient levels can increase yields and reduce by-product formation.
- **Ethylene Recycling:** Recycling unreacted ethylene from the reactor outlet back into the feed stream minimizes raw material waste. Implementing high-efficiency separation techniques, like selective membranes, ensures the maximum recovery of unreacted ethylene.

- **Oxygen Recovery:** Improved oxygen recovery from reactor effluent, using pressure swing adsorption or other separation techniques, can reduce oxygen consumption and lower costs.

- **Closed-Loop Systems:** Implementing a closed-loop system for waste gases and by-products can reduce emissions and improve feedstock efficiency. Capturing and reusing heat from exothermic reactions further improves overall energy efficiency.

7 References

- Bruns, B., Grünewald, M., Riese, J. (2020). Analysis of capacity potentials in continuously operated chemical processes. *Chemie Ingenieur Technik, 92*(12), 2005-2015. https://doi.org/10.1002/cite.202000053

- Rebsdat, S., Mayer, D. (2001). Ethylene Oxide. In *Ullmann's Encyclopedia of Industrial Chemistry* (Vol. 13). Wiley-VCH. https://doi.org/10.1002/14356007.a10117