Process Development for the Production of Mono Propylene Glycol

Mr. Ivica MARJANOVIC
UPMC – Université Pierre et Marie Curie, Paris – CAPGEMINI, Paris

Background & Description:

This project focuses on the simulation and preliminary design of a chemical process for the production of Mono Propylene Glycol (MPG) from Propylene Oxide (PO) using Aspen HYSYS, a widely used process simulation tool in the chemical industry.

MPG ($C_3H_8O_2$) is a colorless, odorless liquid used extensively in the manufacture of unsaturated polyester resins, antifreeze, food and pharmaceutical products, and cosmetics. Its industrial production is typically achieved via hydration of propylene oxide, a process that can proceed via non-catalyzed or catalyzed pathways.

The chemical reaction considered is:

C5H6O + H2O → C3H8O2

In this study, the simulation assumes non-catalyzed vapor-phase hydrolysis, with a conversion rate of 90% for propylene oxide at a reactor temperature of 200°C and a pressure of 1 bar.

The process is composed of the following main steps:

1. **Mixing & Preheating:** Propylene oxide and water are pumped from storage and mixed in a buffer tank. The feed is preheated to 200°C.
2. **Reaction (Conversion Reactor):** The preheated mixture enters a vapor-phase conversion reactor, where 90% of the PO is converted into MPG.
3. **Distillation:** The reactor output is sent to a distillation column designed to recover:
    - *Top stream:* Unreacted PO, water, and minor traces of MPG.
    - *Bottom stream:* Purified MPG (product stream).
4. **Cooling & Storage:** The purified product is cooled to ambient conditions and stored.

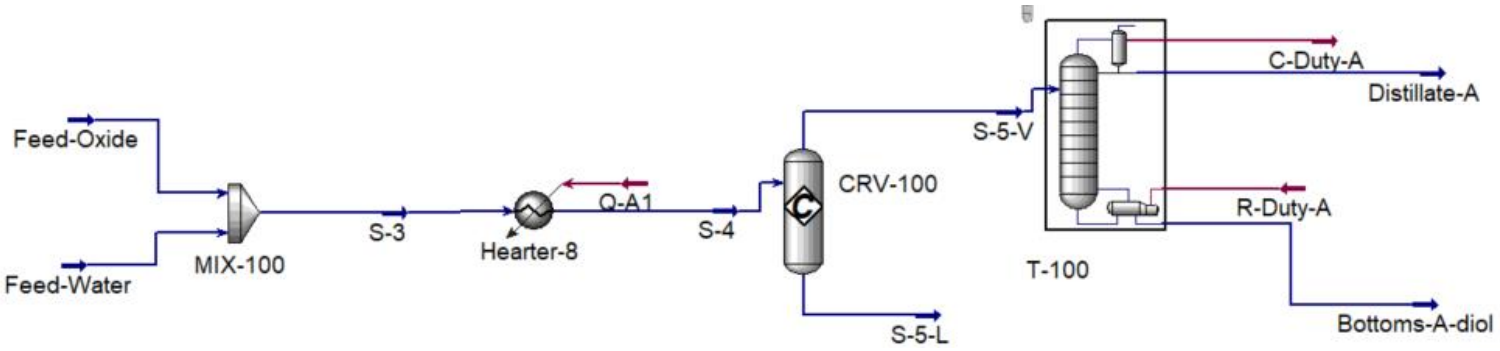
The simulation achieved the production of 16.42 kmol/h of MPG, corresponding to 30 TPD (tons per day) of product. The conversion reactor operated steadily at the target conditions, and the distillation column efficiently separated the components, with MPG recovered at a high purity in the bottom stream.

This study illustrates that Aspen HYSYS is a powerful and reliable platform for the simulation and optimization of industrial chemical processes. The simulation results align well with previously reported work performed using DWSIM, showing comparable performance in process design and parameter estimation.

Furthermore, the integration of kinetic data from literature (e.g., Kozlovsky et al., 2002) enables more realistic modeling of the reaction, offering a path toward future improvements, including side-product formation (DPG, TPG) and catalytic scenarios.

Thermodynamic package: The NRTL thermodynamic model was selected for its high accuracy in modeling non-ideal polar mixtures, especially systems involving water-organic interactions, such as those in PO/H_2O/MPG systems.

Flowsheet



Results:

Master Property Tableau								
Object	**Feed-Oxide**	**Feed-Water**	**S-3**	**S-4**	**S-5-V**	**S-5-L**	**Distillate-A**	**Bottoms-A-diol**
T (°C)	**25**	**25**	**25**	**200**	**657.7**	**657.7**	**36.84**	**184.5**
P (bar)	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**
Molar Flow (kgmole/h)	**20.56**	**20.56**	**41.12**	**41.12**	**22.62**	**0**	**3.940**	**18.68**
Mole Fract (12-C3diol)	**0**	**0**	**0**	**0**	**0.8182**	**-**	**0**	***0.9908***
Mole Fract (12C3Oxide)	**1**	**0**	**0.5**	**0.5**	**0.0909**	**-**	**0.5218**	**0**
Mole Fract (H2O)	**0**	**1**	**0.5**	**0.5**	**0.0909**	**-**	**0.4782**	**0.0092**

Nb : Insignificant quantities (<0) of components in the product streams can be considered negligible, effectively approximating them to zero without impacting the overall process results or conclusions (see flowsheet).

References: Kozlovsky, I. A., et al. (2002). Kinetics and Products Distribution of Selective Catalytic Hydration of Ethylene- and Propylene Oxides in Concentrated Aqueous Solutions. Organic Process Research & Development, 6(5), 660–664. DOI: 10.1021/op010099+