Synthesis of Dimethyl Ether via Methanol Dehydration

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Background & Description:

This project investigates the simulation and optimization of the Dimethyl Ether (DME) production process using the open-source chemical process simulator DWSIM. DME is a versatile chemical compound widely used as a clean fuel, a propellant, and a precursor in chemical synthesis. Its environmentally friendly combustion properties, including low soot and NOx emissions, make it a promising alternative energy source.

The production of DME is based on the dehydration of methanol, governed by the reaction:

2 CH3OH → CH3OCH3 + H2O

This process involves three main steps:

1. **Reaction**: Methanol is converted into DME and water in an adiabatic conversion reactor operating at **15 bars** and **250°C**, achieving a conversion rate of **80%**.
2. **Separation**: The reaction products are separated using two distillation columns:
    - The first column separates DME as a pure top product with a **purity of 99.99%**, while the methanol-water mixture is collected in the bottom stream.
    - The second column recovers unreacted methanol for recycling and isolates water for disposal.
3. **Recycling**: The unreacted methanol is recycled back into the process to maximize efficiency and minimize raw material consumption.

The flowsheet was developed with thermodynamic properties calculated using the **UNIQUAC model**, chosen for its ability to handle complex alcohol-water systems. Simulations achieved a DME production rate of **271.74 kmol/h**.

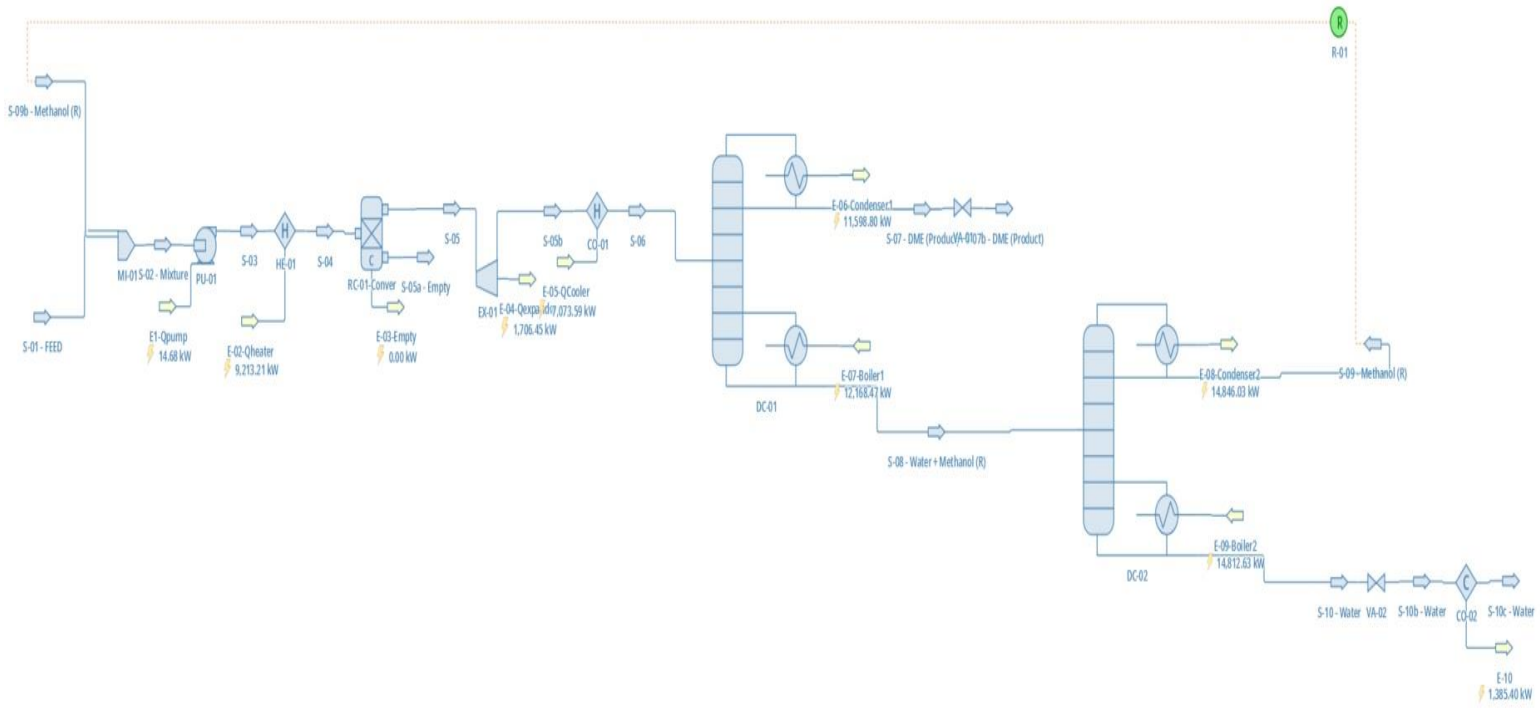
Despite initial challenges in achieving convergence for the distillation columns in DWSIM, adjustments such as optimizing feed plate locations and reflux ratios resolved these issues.

A comparison with Aspen HYSYS simulations shows that DWSIM, while capable of simulating complex processes, may require additional fine-tuning for convergence. These results demonstrate the potential of DWSIM as a robust tool for designing efficient and sustainable chemical processes, particularly in resource-constrained environments.

In parallel, the same process was simulated using **Aspen HYSYS**, yielding **similar results** to those obtained with DWSIM. This demonstrates that **DWSIM** is a powerful open-source tool capable of delivering results comparable to proprietary software like Aspen HYSYS. Its performance highlights DWSIM as a viable and cost-effective alternative for designing and optimizing chemical processes, particularly in resource-constrained environments.

Thermodynamic package: UNIQUAC was chosen as the thermodynamic model because it is better suited and more detailed for systems involving liquid phases. Its equations are particularly applicable to a wide range of mixtures, including those containing water and alcohols.

Flowsheet



Results:

Master Property Tableau								
Object	**S-01-Feed**	**S-02-Mixture**	**S-05**	**S-05a-Empty**	**S-07b-DME(Product)**	**S-08-W+M**	**S-09-M (R)**	**S-10c-W**
T (°C)	**36.88**	**46.73**	**366.19**	**366.19**	**-24.51**	**160.23**	**64.60**	**24.99**
P (kPa)	**101.325**	**101.325**	**1500**	**1500**	**101.325**	**1000**	**101.325**	**101.325**
Molar Flow	**543.48**	**679.35**	**679.35**	**0**	**271.74**	**407.61**	**135.87**	**271.74**
Molar Flow (H2O)	**0**	**<0**	**271.74**	**0**	**<0**	**271.74**	**<0**	**271.74**
Molar Flow (Methanol)	**543.48**	**679.34**	**135.87**	**0**	**<0**	**135.87**	**135.87**	**<0**
Molar Flow (DME)	**0**	**<0**	**271.74**	**0**	**271.74**	**<0**	**<0**	**<0**

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: Müller, M., & Hübsch, U. (2012). Dimethyl Ether. In Ullmann's Encyclopedia of Industrial Chemistry (Vol. 11, pp. 305–308). Wiley-VCH Verlag GmbH & Co. KGaA. DOI: 10.1002/14356007.a08_541.