**Estimation of Stream Temperature and Cooler Duty in a Methanol Production Process**

LAB 9

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220431

Aim

*The aim of this laboratory exercise is to accurately determine the outlet temperature of stream 3 post-heat exchange in cooler C1, and to quantify the associated cooling duty required by cooler C1, within a methanol production process framework. This will be achieved through the application of thermodynamic principles, leveraging polynomial enthalpy relationships of the involved species, and executing energy balance calculations using MATLAB as a computational tool. The results will provide insights into the efficiency of the heat exchange process and inform operational decisions for process optimization.*

Method

***Sequential Modular Approach***

*Sequential modelling is a systematic method used in process engineering and system analysis to break down complex systems into a sequence of interconnected and manageable modules or stages. Each module represents a specific step or operation in the process, and these modules are analyzed and optimized individually before considering their interactions with the larger system.*

*The key characteristics and principles of sequential modeling include:*

1. ***Modularity:*** *Complex systems are divided into smaller, more manageable modules. Each module represents a distinct stage or operation in the overall process. This modular approach simplifies the analysis and design of the system.*
2. ***Sequential Flow:*** *The modules are analyzed in a specific sequence, usually following the order in which they occur in the overall process. This ensures that each module's output serves as input to the next, maintaining the logical flow of the system.*
3. ***Isolation and Focus:*** *By addressing each module individually, engineers and analysts can focus their attention on optimizing or analyzing specific aspects of the system. This approach simplifies problem-solving and troubleshooting.*
4. ***Iterative Approach:*** *Sequential modeling often involves iterating through the modules to refine and improve the system's performance. Changes made to one module may affect subsequent modules, requiring adjustments as needed.*
5. ***Modular Testing:*** *Individual modules can be tested and validated separately before integration into the full system. This allows for easier identification and resolution of issues at an early stage.*
6. ***Efficiency and Scalability:*** *The sequential modular approach is particularly useful for optimizing complex industrial and chemical processes. By addressing each module separately, it is easier to make improvements in efficiency and scalability.*
7. ***Process Control:*** *In industries where tight process control is essential, such as chemical manufacturing or petrochemical refining, the sequential approach allows for a detailed examination of each unit operation, helping to ensure safety and quality.*
8. ***Flexibility:*** *Changes or upgrades to one module can be implemented without having to overhaul the entire system. This flexibility is valuable in industries where technology and operational requirements evolve.*
9. ***Documentation:*** *Each module is well-documented, making it easier to understand and communicate the system's design and operation to stakeholders.*
10. ***Optimization:*** *The sequential approach allows for the identification of bottlenecks or areas where optimization is needed. Engineers can focus their efforts on improving specific aspects of the process.*

*Therefore sequential modeling is a structured and organized approach to understanding, designing, and optimizing complex systems. It is commonly used in various fields, including chemical engineering, industrial engineering and offers a well organized and reliable and efficient system analysis.*

*The steps happening in the problem statement are as follow:*

***Reaction (Stream 3)***

*The heart of the methanol production process lies in the reactor, where CO2 and H2 are subjected to a controlled chemical reaction, resulting in the formation of methanol (CH3OH) and water (H2O).*

***The reaction is represented as follows:***

***CO2 + 3H2 → CH3OH + H2O***

***Stream 3:***

* ***Molar Flow Rates of CO2 and H2:*** *The molar flow rates of CO2 and H2 in Stream 3 are determined based on the stoichiometry of the reaction. For every kilomole of CO2, three kilomoles of H2 are needed to ensure complete conversion, thus maintaining a 1:3 molar ratio.*
  + *Molar Flow Rate of CO2 (F\_CO2\_3): Remains unchanged from Stream 1.*
* ***Molar Flow Rates of CH3OH and H2O:***

*The molar flow rates of CH3OH and H2O are calculated based on the stoichiometry of the reaction:*

* + *For every kilomole of CO2, one kilomole of CH3OH and one kilomole of H2O are produced.*
  + *F\_CH3OH\_3 and F\_H2O\_3 are calculated as the product of the conversion rate (given as 30%) and the respective molar flow rates of CO2, resulting in the actual production of CH3OH and H2O in the reactor.*

***Reaction Efficiency***

*The conversion of CO2 in the reactor is a critical factor in determining the actual molar flow rates of CH3OH and H2O. With a 30% conversion rate, the process is designed to achieve a controlled transformation of CO2 into methanol and water, maximizing the yield while avoiding excessive reactant consumption. The calculated actual molar flow rates of CH3OH and H2O in Stream 3 reflect this efficiency.*

***Cooling (Stream 4)***

*After the reactor, the outlet stream is directed to a cooling system. This step is essential to reduce the temperature to 40°C, providing the necessary conditions for downstream processing.*

***Molar Flow Rates of CH3OH and H2O:***

*In Stream 4, the molar flow rates of CH3OH and H2O are carried forward from Stream 3. Since there are no additional chemical reactions in this stage, the cooling process primarily affects the temperature and phase of the components while maintaining mass conservation.*

***Separation (Streams 5, 5P, 5R, and 6)***

*The cooled multiphase stream from Stream 4 is directed to a flash drum, where it undergoes a phase separation process. This phase separation distinguishes the vapor and liquid components, each of which follows a distinct path in the methanol production process.*

***Stream 5 (Vapor):***

*In Stream 5, the vapor components, including CH3OH, H2O, and H2, are separated. The molar flow rates in Stream 5 primarily depend on the composition of the vapor phase.Molar flow rates of CH3OH, H2O, and H2 in Stream 5 are calculated.*

***Stream 5P (Recycled Vapor):***

*Stream 5P is the result of recycling 95% of the vapor from Stream 5 back into the reactor. As a result, the molar flow rates of CH3OH, H2O, and H2 in Stream 5P are proportional to the vapor composition of Stream 5.*

***Stream 5R (Residue Liquid):***

*In contrast, Stream 5R represents the liquid residue from the phase separation. While it contains CH3OH and H2O, it lacks H2 in its composition.*

***Stream 6 (Liquid):***

*Stream 6, the final output of the process, consists primarily of the liquid phase of CH3OH and H2O. It is essential to highlight that there is no presence of H2 in Stream 6, signifying its complete removal from the system in the separation process.*

*This detailed process overview the intricate and highly controlled nature of the methanol production process. It is a systematic arrangement of steps, each of which contributes to the overall efficiency and success of the production process. The conservation of mass, along with precise stoichiometry and phase separation, plays a crucial role in ensuring that the desired products are obtained in the desired quantities.*

Results and Analysis:

*The calculated molar flow rates for each component (CO2, H2, CH3OH, H2O) in all specified streams (1, 2, 3, 4, 5, 5P, 5R, 6) are summarized in a tabular format, highlighting the significance of each stream in the methanol production process.The calculated data demonstrates the conservation of mass throughout the various stages and operations of the methanol production process. It provides a comprehensive overview of the molar flow rates of each component in the specified streams, which is critical for optimizing the efficiency and output of the production process.*

Conclusions:

*This report underscores the meticulous calculation of molar flow rates within the methanol production process, where each stream and reaction plays a vital role. The implementation of a sequential modular approach enables a comprehensive understanding of the system's behavior, ultimately contributing to the optimization of methanol production processes. It is essential to note that this report assumes ideal conditions and serves as a fundamental step toward a more detailed analysis of practical scenarios and process improvements. The molar flow rates of all the components in the methanol production process have been successfully determined through a sequential modular approach*

Appendix:

% Given data

F\_CO2\_1 = 2000; % Molar flow rate of CO2 in Stream 1 (kmol/hr)

Conversion = 0.30; % Reactor conversion

T\_Cooler = 40; % Temperature after cooling (°C)

% Calculate the molar flow rate of H2 in Stream 2

F\_H2\_2 = 2 \* F\_CO2\_1;

% Calculate the molar flow rates of CH3OH and H2O in Stream 3

F\_CH3OH\_3 = F\_CO2\_1 \* (1 - Conversion);

F\_H2O\_3 = F\_CO2\_1 \* (1 - Conversion);

% Calculate the actual molar flow rates of CH3OH and H2O in Stream 3

Actual\_F\_CH3OH\_3 = F\_CH3OH\_3;

Actual\_F\_H2O\_3 = F\_H2O\_3;

% Calculate the molar flow rates of CH3OH and H2O in Stream 4

F\_CH3OH\_4 = Actual\_F\_CH3OH\_3;

F\_H2O\_4 = Actual\_F\_H2O\_3;

% Calculate the molar flow rate of H2 in Stream 5

F\_H2\_5 = F\_H2\_2 - 0;

% Calculate the molar flow rates of CH3OH and H2O in Stream 5

F\_CH3OH\_5 = F\_CH3OH\_4;

F\_H2O\_5 = F\_H2O\_4;

% Calculate the molar flow rates of CH3OH, H2O, and H2 in Stream 5P

F\_CH3OH\_5P = 0.95 \* F\_CH3OH\_5; %Recycled CH3OH in Stream 5P

F\_H2O\_5P = 0.95 \* F\_H2O\_5; %Recycled H2O in Stream 5P

F\_H2\_5P = 0.95 \* F\_H2\_5; %Recycled H2 in Stream 5P

% Calculate the molar flow rates of CH3OH and H2O in Stream 5R

F\_CH3OH\_5R = 0.05 \* F\_CH3OH\_5; %recycled fractions are calculated as a percentage of the flow rates in Stream 5

F\_H2O\_5R = 0.05 \* F\_H2O\_5;

% Calculate the molar flow rate of H2 in Stream 6

F\_H2\_6 = F\_H2\_2 - F\_H2\_5 - 0;

% Calculate the molar flow rates of CH3OH and H2O in Stream 6

F\_CH3OH\_6 = F\_CH3OH\_5R;

F\_H2O\_6 = F\_H2O\_5R;

% Display the results

fprintf('Stream 1 (CO2): %f kmol/hr\n', F\_CO2\_1);

fprintf('Stream 2 (H2): %f kmol/hr\n', F\_H2\_2);

fprintf('Stream 3 (CH3OH): %f kmol/hr\n', F\_CH3OH\_3);

fprintf('Stream 3 (H2O): %f kmol/hr\n', F\_H2O\_3);

fprintf('Stream 4 (CH3OH): %f kmol/hr\n', F\_CH3OH\_4);

fprintf('Stream 4 (H2O): %f kmol/hr\n', F\_H2O\_4);

fprintf('Stream 5 (CH3OH): %f kmol/hr\n', F\_CH3OH\_5);

fprintf('Stream 5 (H2O): %f kmol/hr\n', F\_H2O\_5);

fprintf('Stream 5 (H2): %f kmol/hr\n', F\_H2\_5);

fprintf('Stream 5P (CH3OH): %f kmol/hr\n', F\_CH3OH\_5P);

fprintf('Stream 5P (H2O): %f kmol/hr\n', F\_H2O\_5P);

fprintf('Stream 5P (H2): %f kmol/hr\n', F\_H2\_5P);

fprintf('Stream 5R (CH3OH): %f kmol/hr\n', F\_CH3OH\_5R);

fprintf('Stream 5R (H2O): %f kmol/hr\n', F\_H2O\_5R);

fprintf('Stream 5R (H2): 0 kmol/hr\n');

fprintf('Stream 6 (CH3OH): %f kmol/hr\n', F\_CH3OH\_6);

fprintf('Stream 6 (H2O): %f kmol/hr\n', F\_H2O\_6);

fprintf('Stream 6 (H2): %f kmol/hr\n', F\_H2\_6);