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# PROCESS DESIGN AND SIMULATION OF GREEN METHANOL PRODUCTION AND ECONOMIC ASSESSMENT

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MASTER'S DISSERTATION PRESENTED
TO FACULDADE DE ENGENHARIA DA UNIVERSIDADE DO PORTO IN
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Master in Chemical Engineering

# *Process Design and Simulation of Green Methanol Production and Economic Assessment*

## Master dissertation

Of

Vasco Araújo

**Developed within the course of dissertation**

held in

**The Navigator Company**


Supervisor at FEUP: **Prof. Adélio Mendes**

Joint supervisor at FEUP: **Prof. Fernando Martins**

Coordinator at The Navigator Company: **Eng. Alexandre Gaspar**



**July 2021**

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# Abstract

The current climate emergency begets swift and effective measures to drastically decrease carbon emissions: there is urgent need to develop feasible and safe ways to store and distribute energy from renewable sources.

One approach that has been given some discussion in recent years is the usage of methanol. Methanol, primarily produced from fossil-fuel-based synthetic gas, can also be synthesized from the direct carbon dioxide hydrogenation. This allows hydrogen to be safely stored in methanol, a critical energy vector and feedstock, while giving a good use to biogenic carbon dioxide from industrial effluents or captured from the atmosphere. Literature shows that green methanol can be produced cost effective from green hydrogen and biogenic $CO_2$.

Utilizing the simulation software Aspen Plus V12, the present work studies the efficiency and economic viability of different process configurations for methanol synthesis via direct $CO_2$ hydrogenation compared with the conventional process, based on natural gas. The impact of different key factors in the methanol unit production cost, namely the use of an innovative bifunctional catalyst, as well as the cost of fossil versus green methanol production, is analysed.

The obtained results indicate that the most competitive green methanol processes use either a single reactor with a recycle stream, or two reactors in series with a recycle stream. The cost of the produced methanol for both process configurations is the same as it is 375 €/ton. Further economic analysis shows that the methanol production cost is dictated primarily by the cost of hydrogen, which accounts for ca. 80% of the green methanol cost structure; the cost of $CO_2$ accounts for ca. 8% of the green methanol cost structure. The comparison between fossil methanol and green methanol shows that green methanol reaches the break-even point by 2025.

**Keywords:** methanol, process simulation, carbon dioxide hydrogenation, economic analysis, process configurations comparison

# Resumo

A atual emergência climática obriga a medidas rápidas e efetivas de forma a diminuir drasticamente emissões de carbono: existe uma necessidade urgente de desenvolver formas viáveis e seguras de armazenar e distribuir energia proveniente de fontes renováveis.

Recentemente, uma abordagem que tem sido objeto de discussão é a utilização de metanol. Metanol, produzido principalmente através de gás de síntese à base de combustíveis fosseis, também pode ser sintetizado através da hidrogenação direta de dióxido de carbono. Isto permite que o hidrogénio seja armazenado em segurança no metanol, um vetor energético crítico e matéria-prima, enquanto, ao mesmo tempo, dá um bom uso ao dióxido de carbono biogénico de efluentes industriais ou capturado da atmosfera. A literatura mostra que o metanol verde pode ser produzido de forma rentável a partir de hidrogénio verde e dióxido de carbono biogénico.

Utilizando o software de simulação Aspen Plus V12, o presente trabalho estuda a eficiência e viabilidade económica de diferentes configurações processuais para síntese de metanol via hidrogenação direta do CO2 em comparação com o processo convencional, baseado no gás natural. É analisado o impacto de diferentes fatores-chave no custo de produção por unidade de metanol, nomeadamente o uso de um catalisador bifuncional inovador, bem como o custo da produção de metanol fóssil versus metanol verde.

Os resultados obtidos indicam que os processos de metanol verde mais competitivos utilizam um único reator com uma corrente de reciclagem, ou dois reatores em série com uma corrente de reciclagem. O custo de produção por unidade de metanol é semelhante para ambas as configurações, sendo este 375 €/t. Adicionalmente, a análise económica mostra que o custo de produção do metanol é ditado principalmente pelo custo do hidrogénio, que é responsável por ca. 80% da estrutura de custos do metanol verde; o custo do CO2 é responsável por ca. 8% da estrutura de custos do metanol verde. A comparação entre metanol fóssil e metanol verde mostra que o metanol verde atinge o ponto de *break-even* até 2025.

**Palavras-chave:** metanol, simulação de processos, hidrogenação de dióxido de carbono, análise económica, comparação entre configurações processuais

# Declaration

I hereby declare, under word of honour, that this work is original and that all non-original contributions is indicated and due reference is given to the author and source

Vasco Araújo

*July, 2021*

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Notation and Glossary

| | | |
|---|---|---|
| $A$ | area | $m^2$ |
| $k_A$ | Reaction rate constant for reaction *i* | |
| $K_A$ | Equilibrium constant for reaction *i* | |
| $K_j$ | Adsorption constant for species *j* | 1/bar |
| $f_j$ | Fugacity for species *j* | bar |
| $r_i$ | Rate expression for reaction *i* | |
| $R$ | Gas constant = 8.314 | J/mol.K |

*Greek Letters*

| | | |
|---|---|---|
| $\Delta H$ | Enthalpy change | kJ/mol |

*Indexes*

| | |
|---|---|
| *i* | Reaction *i* |
| *j* | Component species *j* |

***Abbreviations***

| | |
|---|---|
| MeOH | Methanol |
| RWGS | Reverse Water-Gas Shift reaction |
| Conv | Conventional Process |
| LHHW | Langmuir-Hinshelwood-Hougen-Watson kinetics |

# 1 Introduction

## 1.1 Framing and presentation of the work

Methanol is a key feedstock for the chemical industry, being one of the four major chemicals, alongside ethylene, ammonia and propylene, and is becoming a reference fuel. It is used in the production of other chemicals such as acetic acid, formaldehyde and plastics. Methanol can also be used as a fuel – either by itself, as a blend with gasoline, for the production of biodiesel, but as a feedstock of critical fuels such as jet fuel and marine fuel.

The first commercial methanol synthesis plant was built by BASF, in 1923, with a process running at 300 ºC and 300 bar. Due to the high temperature and pressure requirements, a new catalyst was developed which required less extreme conditions. Conventionally, methanol is produced from synthesis gas, and the introduction of a $CuO/ZnO/AL_2O_3$ catalyst allowed for the synthesis of methanol at operating conditions of 200-300 ºC and 50-100 bar (IRENA, 2021).

IRENA (2021) shows that methanol production accounts for around 10% of $CO_2$ emissions by the chemical and petrochemical sector. Therefore, addressing emissions from methanol synthesis is a key component for decarbonisation of the chemical sector, and possibly the transport sector as well.

While the worldwide annual production of methanol was about 98 Mt in 2019, renewable methanol synthesis accounted for less than 0.2 Mt. Methanol demand is expected to increase, to reach more than 120 Mt by 2025 and 500 Mt by 2050 (IRENA, 2021).

Methanol is produced almost exclusively from fossil fuels. However, methanol can also be made from biomass feedstocks (from forestry and agricultural waste and by-products to black liquor from the pulp and paper industry). Green methanol can also be synthesized from $CO_2$ captured from air or biogenic and green hydrogen.

In the past decades, methanol production from carbon dioxide and hydrogen (called carbon dioxide hydrogenation) was proposed as a green chemical process, which addresses $CO_2$ emissions from methanol synthesis. The cost of methanol production from carbon dioxide hydrogenation is higher than the cost of fossil methanol, due mostly to the price of pure hydrogen feed.

Regardless of the route of synthesis, green methanol is chemically identical to methanol produced from fossil fuel sources, allowing direct replacement of fossil methanol in all of its current uses. Olah (2005), laureate nobel prize of chemistry in 2005, proposes a “methanol economy” as a more practical approach compared to the widely discussed “hydrogen

economy". Existing liquid fuel infrastructure (pipelines and tanks) could be used with little modification, and the safety concerns associated with hydrogen can be avoided.

A study by Kiss et al. (2016) of operating conditions of the reactor for methanol synthesis via carbon dioxide hydrogenation reported that high operating pressure at a temperature range of 230-260 ºC, as well as an increase in reactant ratio ($H_2$:$CO_2$) directly correlated to improved reactant conversion to methanol. Borisut and Nuchitprasittichai (2020) performed simulation-based optimization, aiming to minimize the cost of methanol production via $CO_2$ hydrogenation, comparing different process configurations.

The aim of this thesis is the design and simulation of methanol synthesis through carbon dioxide hydrogenation, not only for different process configurations, but also for two different catalysts - a highly active Cu/Zn/Al/Zr fibrous catalyst and an experimental catalyst comprehending active sites for the methanol synthesis and for the reverse water gas shift reaction. Also, a simulation of the conventional process of methanol synthesis from synthetic gas was made, allowing for a comparison to be drawn between all simulations. Finally, an economic analysis was made for each design and to measure the impact of different process variables in the methanol production cost.

## 1.2 The Navigator Company

The Navigator Company is an integrated forest producer, whose end products are pulp and paper, tissue, and energy. Its operations are based at modern, large-scale industrial units that use state-of-the-art technology and are a benchmark for quality in the sector.

Navigator (2021) is Europe's largest manufacturer of uncoated woodfree printing and writing paper, and the sixth largest in the world, pursuing a successful strategy of innovation and developing its own brands and premium products.

Currently, Navigator produces annually nearly 1.6 million tons of paper, 1.5 million tons of pulp each year, of which roughly 80% is integrated into paper production, and 2.5 TWh of electricity per annum. In Portugal, ca. 5% of all electricity is generated from The Navigator Company.

Aiming to be a global company, admired for their innovative and sustainable way of business that contributes to people's wellbeing, Navigator is a company of integrity, excellence and sustainability, and an ambassador for Portuguese quality around the world.

## 1.3 Contribution of the author to the work

The reported work was completed in its entirety by the author, Vasco Araújo.

## 1.4 Organization of the dissertation

The rest of this dissertation is organized as follows: In Chapter Two, we present background information in the form of a brief historical perspective of methanol synthesis, and the literature that influenced the current work. Chapter Three discusses the software used, as well as all information regarding the catalysts and reaction kinetics. In Chapter Four, a simulation of the conventional process for methanol synthesis from synthetic gas is shown, followed by the studied process configurations. Key process parameters are explicit, followed by an insight into the usage of utilities and the Heat Integration for all processes, along with an economic analysis for each process configuration. The economic analysis continues, studying the impact of key process variables in the overall methanol production cost, as well as a cost comparison between fossil methanol and green methanol in the upcoming years. Finally, Chapter Five presents the conclusions and future work, with Chapter Six showing an assessment of the work done.

# 2 Context and State of the art

Methanol synthesis has been extensively studied in the scientific literature. Several kinetic models have been reported, for different catalysts, reaction conditions and feedstock composition. Many models consider the methanol synthesis from syngas , while others consider the direct hydrogenation of $CO_2$, reporting different kinetic models and laws.

The work by Grabow and Mavrikakis (2011) reports a microkinetic model assuming different intermediates involved in methanol synthesis from syngas. Interestingly, two thirds of synthesized methanol is produced from the hydrogenation of carbon dioxide. Kunkes et al. (2015) discussed whether methanol synthesis and RWGS are parallel pathways, methanol synthesis proceeds forcefully by a "two-step" reaction - sequential RWGS followed by carbon monoxide hydrogenation, or whether methanol synthesis and RWGS share a common intermediate. These authors concluded that the first hypothesis is the correct one, the methanol synthesis involves parallel pathways.

Some studies, concerning macrokinetic models with explicit rate laws, were developed by Graaf et al. (1986, 1990). Taking into account the involved reactions of carbon monoxide hydrogenation, reverse water-gas shift and carbon dioxide hydrogenation, Graaf et al. developed a kinetic model based on an LHHW mechanisms, over a commercial $CuO/ZnO/Al_2O_3$ catalyst from Haldor Topsoe. The determined rate laws assume two different active sites, with carbon monoxide and carbon dioxide adsorbing competitively on the metallic copper site, and hydrogen and water adsorbing competitively on the zinc oxide site. The reaction models by Graaf et al. (1988) were used the present work.

An exhaustive experimental study on the chemical equilibrium in methanol synthesis and water gas shift reaction was developed by Graaf et al. (1986), studying fixed-bed catalytic reactor at a pressure range of 10-80 bar and a temperature range of 200-270 ºC. According to Graaf et al., 1990, a comparison with previously reported studies showed that the best results are obtained with the Soave-Redlich-Kwong equation of state. The difference between it and the Peng-Robinson equation state (Peng and Robinson, 1976) was not significant, however, the equation fits better to the experimental results than other equations, such as the Redlich-Kwong equation (Redlich and Kwong, 1949) and the Lewis and Randall rule (Lewis and Randall, 1923).

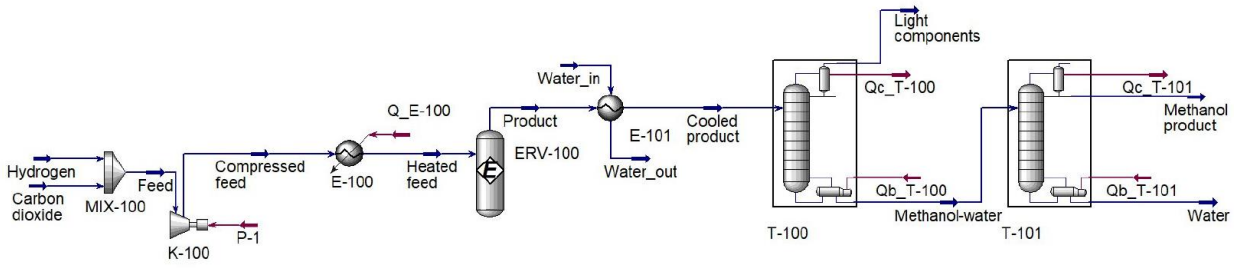
As previously mentioned, the exothermicity of the process and the decrease in stoichiometry during the reaction implies the need for low process temperatures and high pressures. Under normal synthesis conditions (75 bar, 225 ºC), carbon conversion in traditional gas reactors cannot overcome the thermodynamic limit of about 60% (Dybkjaer et al., 2006).

Two main types of reactors are used today in methanol synthesis: adiabatic and isothermal, with their use differing with the chosen working conditions. Slurry reactors are used for liquid phase synthesis of methanol, but to a much lesser extent.

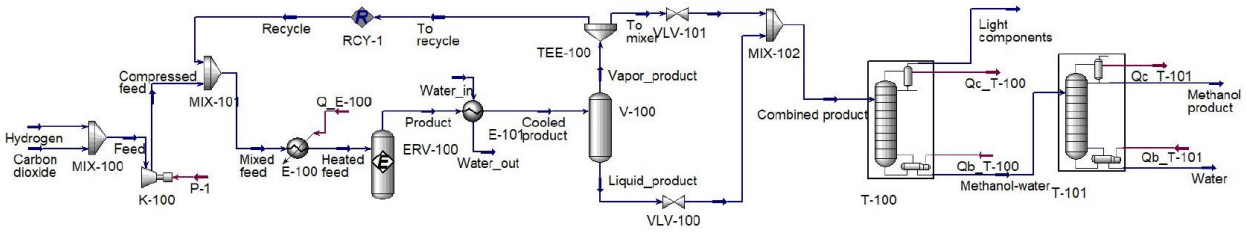
In this work, an isothermal reactor was considered. Isothermal reactors work primarily as a heat exchanger, in which cooling is achieved by water circulation on the mantle of the tube bundle. These systems enable high conversion and low catalyst volume; however, temperatures need to reach 240 – 260 ºC, with a high recycle ratio. Such reactors were developed and customized by several industries, such as Topsoe (Lahne and Lohmüller, 1986) and Mitsubishi Heavy Industries (Shimomura and Nojima, 1988).

The work by Kiss et al. (2016) proposed an efficient process for carbon dioxide hydrogenation to methanol with a Cu/Zn/Al/Zr catalyst, with a stripping unit where wet hydrogen (saturated with water) flowed in counter-current with the reaction products, removing $CO_x$ from the reaction products while also removing water from the wet hydrogen feed. The present work utilizes the reaction kinetics provided by Kiss et al..

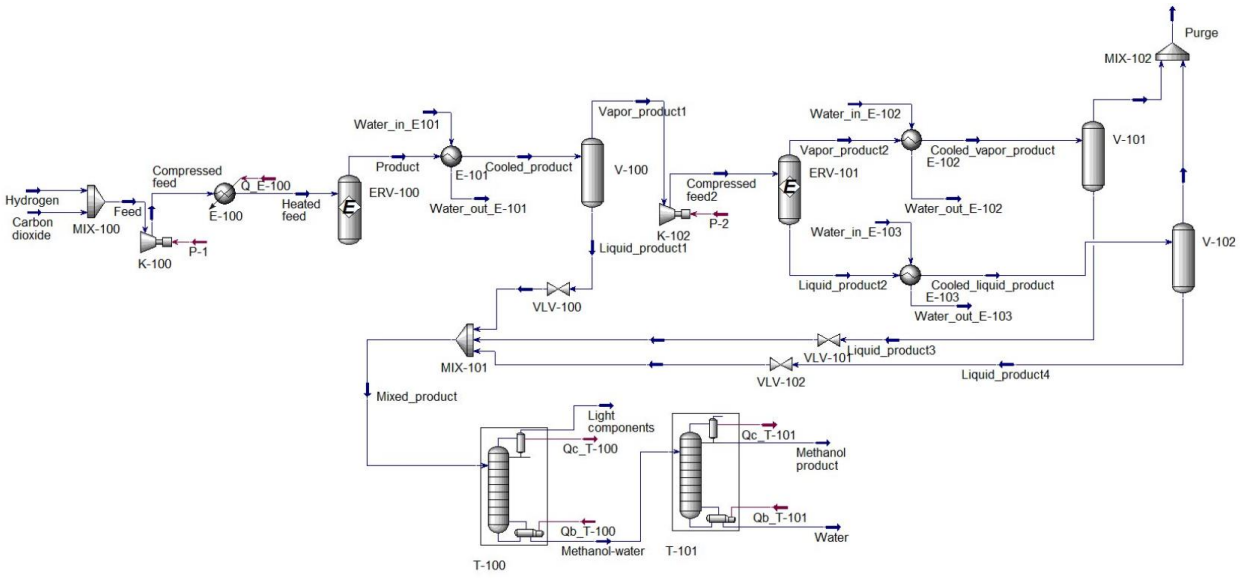
Borisut and Nuchitprasittichai (2020) studied different process configurations for methanol synthesis via direct carbon dioxide hydrogenation: a once-through reactor; a reactor with a recycle stream; and two reactors in series, performing simulation-based optimization, in Aspen HYSYS V10.1, to minimize the cost of methanol production. The study of different process configurations served as basis for the present work:




(a)




(b)




(c)

*Figure 1. Process simulation of methanol production via carbon dioxide hydrogenation: (a) once-through reactor; (b) reactor with recycle; (c) two reactors in series, Borisut and Nuchitprasittichai (2020).*

The current economic landscape for methanol synthesis is changing. In the past, methanol synthesis was easily governed by fossil fuel-based sources. However, trends show that green methanol synthesis will become soon competitive against fossil methanol.

Figure 2 shows a steady increase in methane costs for Europe. This translates into an increase in fossil hydrogen feedstock prices, which, in turn, since methanol synthesis costs is mostly governed by hydrogen feedstock prices, will make fossil methanol more expensive for the foreseeable future.

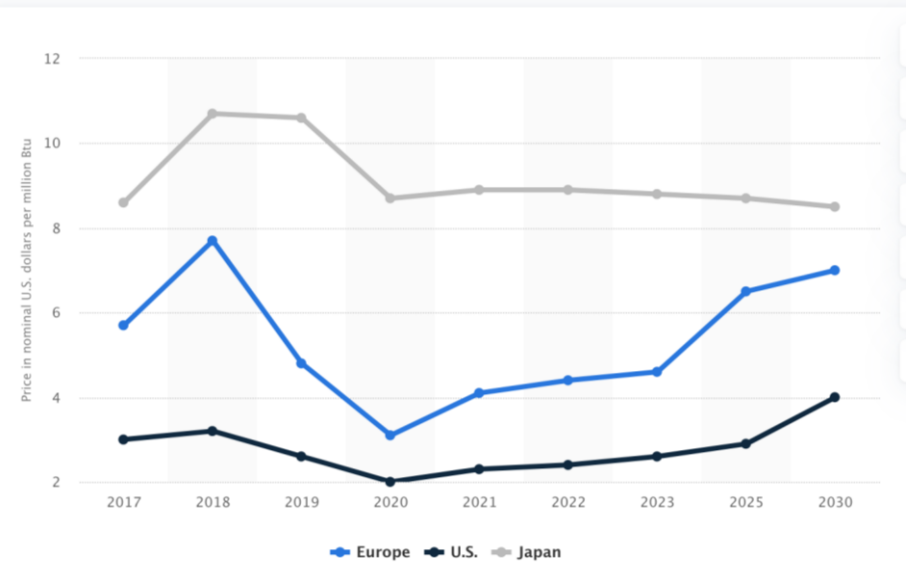



*Figure 2. Natural gas prices in selected markets, from 2017 to 2030, Statista (2021).*

Carbon market price for the European Union shows a drastic increase on the $CO_2$ allowances price now reaching over 55 €/ton (July 2021). Figures 3 and 4 show, respectively, the cost of fossil carbon feedstocks for the year of 2021, and the estimated cost of renewable-sourced carbon dioxide for the year of 2050:

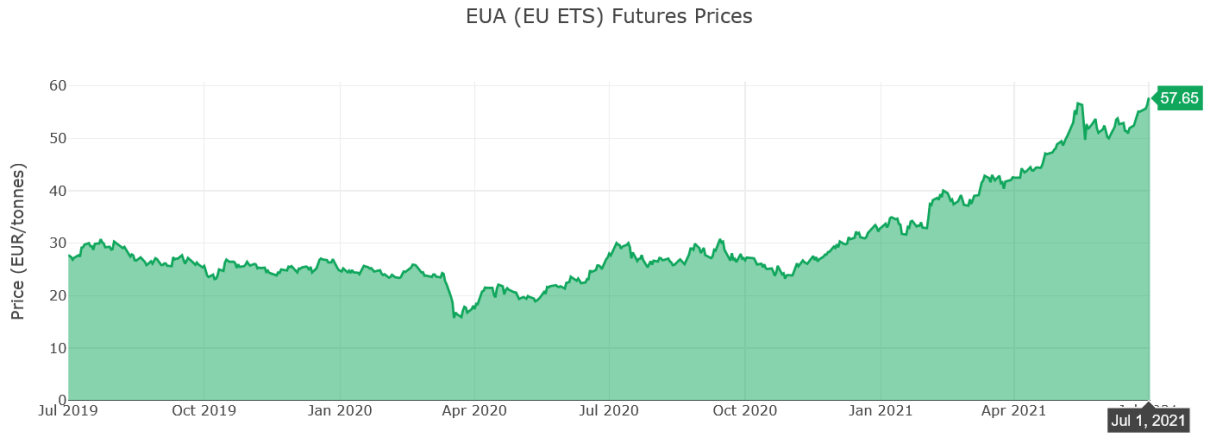



*Figure 3. Carbon market price for the European Union, Ember Climate (2021).*

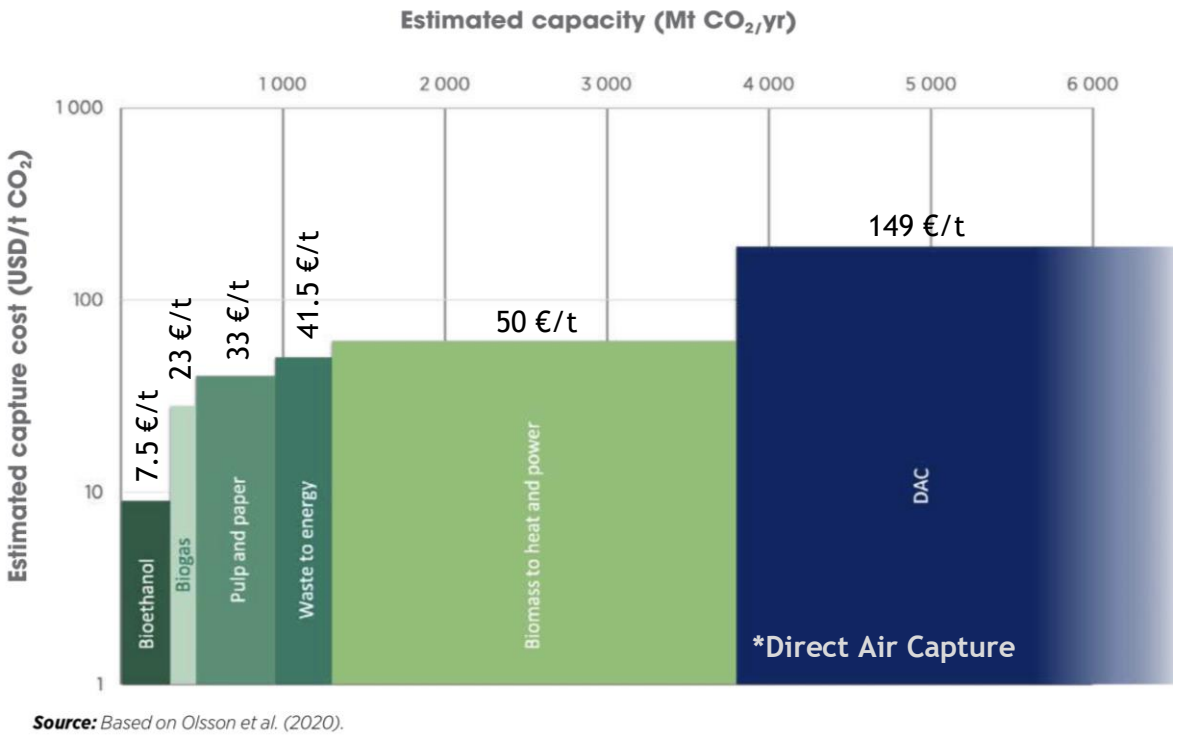



*Figure 4. Estimated renewable-sourced carbon dioxide prices for 2050, IRENA (2021).*

As shown above, except for carbon dioxide sourced from Direct Air Capture, biogenic carbon dioxide will be either competitive or significantly cheaper than the fossil carbon market price. This shift in feedstock prices presents a major economic opportunity to bring forth new and efficient processes, for a cost-competitive production of green methanol.

# 3 Materials and Methods

## 3.1 Computer Application Aspen Plus V12

*Aspen Plus V12* is a chemical process simulator used to mathematically model chemical processes, from unit operations to full chemical plants and refineries. Given a process design and an appropriate selection of thermodynamic models, *Aspen Plus* is able to perform many chemical engineering calculations, including mass and energy balance, vapor-liquid equilibrium, chemical kinetics, mass and heat transfer, among many others. It is used extensively both in industry and academia for steady-state and dynamic simulation, performance modelling, process design and optimization. One of the advantages of this software is its extensive database of species and their pure/binary regressed parameters. It can also handle very complex processes with ease, such as multiple-column separation systems, distillation of chemically reactive compounds, electrolyte solutions, chemical reactors, and complex recycle-bypass streams.

Two features, named “Design Spec” and “Sensitivity Analysis”, were used extensively in this work. The “Design Spec” feature allows the user to automatically vary parameters within user-specified boundaries, in order to achieve the required values. This tool is extremely versatile, allowing for automatic optimization of almost all parameters, from specifying stream purity, to varying the number of tubes in a reactor in order to achieve a desired residence time. The “Sensitivity Analysis” feature is similar to “Design Spec”, differing only in the automatic aspect. While the Design Spec makes changes to the simulation automatically, Sensitivity Analysis allows the user to collect data on varied parameters, for further study and optimization. In short, “Design Spec” allows for automatic optimization, whereas “Sensitivity Analysis” allows for manual optimization.

The Heat Integration was made utilizing the software *Aspen Energy Analyzer*. In terms of the economic analysis, the feature *Aspen Process Economic Analyzer* was used to assess the equipment costs for every configuration.

All configurations were rigorously simulated in *Aspen Plus* using the *RK-Soave* property model, the most suitable for these components ($H_2$, CO, $CO_2$, $H_2O$ and $CH_3OH$) and conditions. Complementary to the chosen property model, the *NRTL* model with Henry components was used in order to accurately model the distillation column, operating at low pressure in which no hydrogen is present (Kiss et al., 2016). All the binary interaction parameters related to the property models are available in the pure components databank of the *Aspen Plus* process simulator.

## 3.2 Reaction Kinetics

The chemistry of methanol synthesis through carbon oxide hydrogenation involves three main reactions:

A) $CO + 2H_2 \leftrightarrows CH_3OH$ $\Delta H_{298\,K} = -90.77$ kJ/mol (1)

B) $CO_2 + H_2 \leftrightarrows CO + H_2O$ $\Delta H_{298\,K} = 41.21$ kJ/mol (2)

C) $CO_2 + 3H_2 \leftrightarrows CH_3OH + H_2O$ $\Delta H_{298\,K} = -49.16$ kJ/mol (3)

Reactions A and C, representing the carbon oxide conversions to methanol are exothermic. As such, a temperature increase in the reactor has a negative impact on equilibrium. Since reaction B, the carbon dioxide conversion to carbon monoxide, is endothermic, a temperature increase impacts positively the equilibrium. Thus, methanol yield is promoted by lower temperatures and higher pressures. This is in line with the work of Kiss et al. (2016). However, due to kinetic limitations at these lower temperatures, an optimal operating region exists, which depends on the hydrogen to carbon dioxide ratio.

In terms of catalyst, Kiss et al. utilize experimental data from An et al. (2009), obtained for a fibrous Cu/Zn/Al/Zr catalyst, designed specifically for the hydrogenation of $CO_2$. The Langmuir-Hinshelwood-Hougen-Watson (LHHW) kinetic model assumes two different active sites – as such, CO and $CO_2$ absorb competitively on the s1-sites, while $H_2$ and $H_2O$ are absorbed competitively on the s2-sites. In the present work, this catalyst is designated as catalyst "A".

The corresponding rate equations for the best kinetic model, out of 48 models tested by Graaf et al. (1988), are:

$$r_{CH_3OH} = k_A \frac{K_{CO}\left(f_{CO}\, {f_{H_2}}^{\frac{3}{2}} - \frac{f_{CH_3OH}}{K_A\sqrt{f_{H_2}}}\right)}{\left(1 + K_{CO}f_{CO} + K_{CO_2}f_{CO_2}\right)\left[\sqrt{f_{H_2}} + \left(\frac{K_{H_2O}}{\sqrt{K_H}}\right) f_{H_2O}\right]} \quad (4)$$

$$r_{CO} = k_B \frac{K_{CO_2}\left(f_{CO_2}\, f_{H_2} - \frac{f_{H_2O}\, f_{CO}}{K_B}\right)}{\left(1 + K_{CO}f_{CO} + K_{CO_2}f_{CO_2}\right)\left[\sqrt{f_{H_2}} + \left(\frac{K_{H_2O}}{\sqrt{K_H}}\right) f_{H_2O}\right]} \quad (5)$$

$$r_{CH_3OH} = k_C \frac{K_{CO_2}\left(f_{CO_2}\, {f_{H_2}}^{\frac{3}{2}} - \frac{f_{H_2O}\, f_{CH_3OH}}{{f_{H_2}}^{\frac{3}{2}}\, K_C}\right)}{\left(1 + K_{CO}\, f_{CO} + K_{CO_2}\, f_{CO_2}\right)\left[\sqrt{f_{H_2}} + \left(\frac{K_{H_2O}}{\sqrt{K_H}}\right) f_{H_2O}\right]} \quad (6)$$

Where $k_A$, $k_B$, and $k_C$ respectively represent the kinetic constants for reactions A, B, and C; $K_A$, $K_B$, and $K_C$ are the equilibrium constants for each reaction; $K_j$ corresponds to the adsorption constant of species $j$; and $f_j$ represents the fugacity of each species $j$. All values and respective units are present in Annex A.

The generalized rate expression to be used in Aspen Plus is given by:

$$r = \frac{(\text{kinetic factor})(\text{driving force expression})}{(\text{adsorption term})} \tag{7}$$

In *Aspen Plus*, the kinetic factor is expressed by $kT^n \cdot \exp\left(-\frac{E_a}{RT}\right)$. All the required input data for the kinetic factor of each reaction is included in Annex A, Table 7 (Kiss et al. 2016, An et al., 2009). It is of note that the units for the pre-exponential constant, driving force expression and adsorption term may vary, therefore may not be the same for all the reactions.

The adsorption term requires re-writing for correct application in *Aspen Plus*, being the same for all reactions (Kiss et al. 2016, Graaf et al., 1988):

$$\left(1 + K_{CO}\, f_{CO} + K_{CO_2}\, f_{CO_2}\right)\left[\sqrt{f_{H_2}} + \left(\frac{K_{H_2O}}{\sqrt{K_H}}\right) f_{H_2O}\right] = \tag{8}$$

$$= \sqrt{f_{H_2}} + \left(\frac{K_{H_2O}}{\sqrt{K_H}}\right) f_{H_2O} + K_{CO}\, f_{CO}\sqrt{f_{H_2}} + \frac{K_{CO}\, K_{H_2O}}{\sqrt{K_H}}\, f_{CO}\, f_{H_2O} + K_{CO_2}\, f_{CO_2}\sqrt{f_{H_2}} + \frac{K_{CO_2}\, K_{H_2O}}{\sqrt{K_H}}\, f_{CO_2}\, f_{H_2O}$$

The adsorption constants are a function of temperature:

$$K_i = a_i \cdot \exp\left(\frac{b_i}{R\,T}\right) \tag{9}$$

However, in *Aspen Plus*, $K$ must be expressed in a logarithmic form. All input parameters are provided in Annex A, Table 8 (Kiss et al. 2016):

$$\ln(K) = A + \frac{B}{T} \tag{10}$$

Kiss et al. configured the LHHW-kinetics in Aspen Plus, testing in a plug flow reactor using equilibrium and kinetics data from literature (An et al. 2009). The comparison between experimental and simulated data showed a good agreement, indicating a correct characterization of the kinetics.

For the hypothetical "B" catalyst, comprehending the methanol synthesis function from $CO_2$ and from CO and a reverse water gas shift function – bifunctional catalyst. Both reaction functions were assumed to follow the models and parameters indicated by Kiss et al. (2016). As such, carbon dioxide would be consumed in two separate pathways: the direct hydrogenation to methanol, and a two-step pathway, converting carbon dioxide to carbon monoxide and

proceeding with carbon monoxide hydrogenation to methanol. This hypothetical catalyst increases carbon dioxide consumption to almost 100% per reactor pass.

In order to establish a point of comparison between the designs and simulations of this work and a regular methanol synthesis facility, which used synthesis gas, a simulation was made following the work of Luyben (2010). However, for the purpose of an apt comparison, the amount of methanol synthesized per year was normalized to 100 kt/y.

For the conventional process, the kinetics used in the work of Luyben (2010) are given by vanden Bussche and Froment (1996), utilizing a solid catalyst. The kinetic LHHW parameters used in the simulation are shown in Table 10, Annex B.

# 4 Results and discussion

## 4.1 Conventional Process

Figure 5 shows the flowsheet for the conventional process, aiming to replicate the work by Luyben (2010); all stream and block summaries are indicated in Appendix C and D, respectively. In this simulation, the RK-Aspen physical property model was used, with exception of the distillation column, where the van Laar equations were used to calculate liquid activity coefficients. Due to inconsistencies within the simulator, assumptions had to be made in order to replicate the reactor block "R1". Thanks to a work by María et al. (2013), it was possible to input correct stream values for the reactor inlet and outlet.

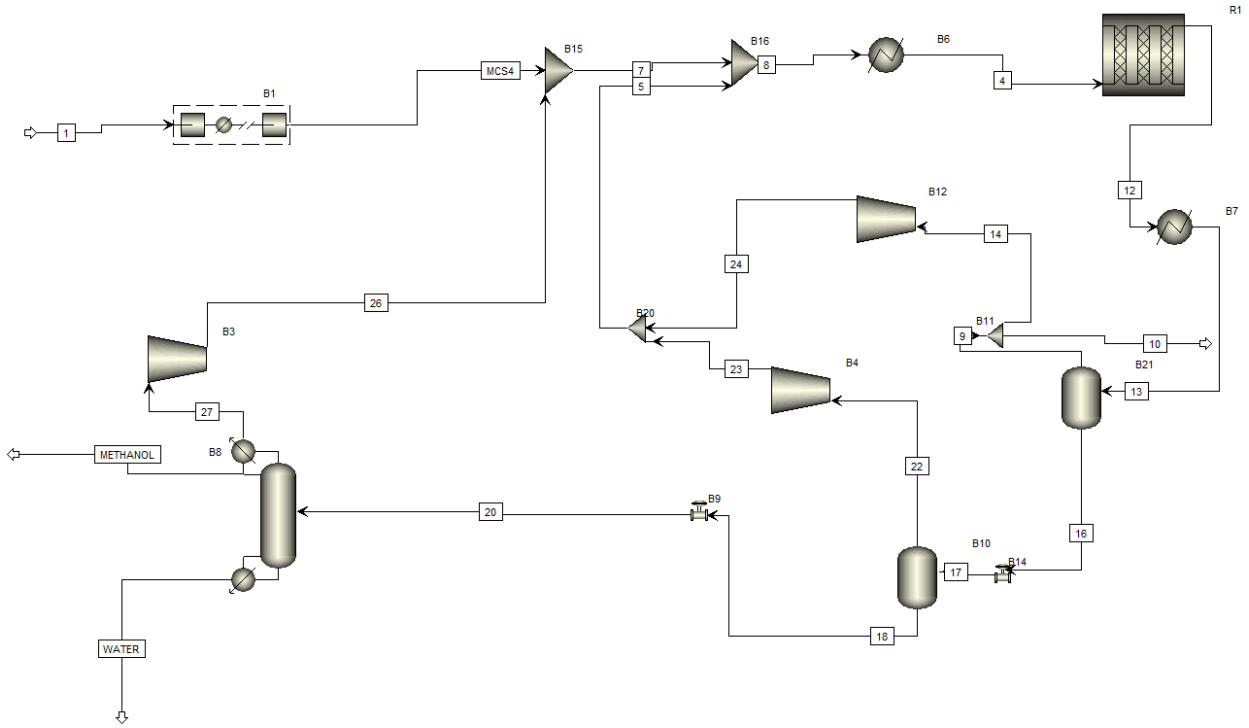



*Figure 5. Process flowsheet for "Conventional Process", replicating the work of Luyben (2010).*

Synthesis gas at 1 bar is compressed in a four-stage compression system to 110 bar. The fresh feed has a $H_2$:CO ratio of 3:1, containing carbon dioxide as well as small amounts of methane and nitrogen, which must be purged.

There are three recycle streams before entering the reactor. The gas is heated to 150 ºC in a reactor preheater. Simulated in *Aspen Plus* using the RPLUG model, the reactor's medium temperature is set at 264 ºC, generating high-pressure steam to cool itself. The reactor has 1710 tubes with length of 12.2 m and a diameter of 0.03675 m.

The reactor effluent is then cooled to 38 ºC. The stream flows into a separator tank operating at 106.5 bar and 38 ºC, with most of the vapor stream being compressed back to 110 bar and recycled. A small molar fraction (0.022) is vented off, removing the inert methane and nitrogen from the system. The inert components, however, are allowed to build up in the system, so that the losses of the reactants in the vent are kept small.

The liquid flowing from the separator tank contains significant amounts of hydrogen, carbon dioxide and methane, due to the high pressure in the separator. These should not be fed directly into the distillation column. As such, a flash tank is used to remove these light components before feeding the stream into the column, operating at 2 bar and 38 ºC. The gas is then compressed to 110 bar and recycled to the reactor.

The liquid effluent is fed into a 42-stage distillation column, at stage 27, which operates at 1 bar, with a reflux ratio of 1.00 and a fixed reflux-drum temperature of 50 ºC. A small vapor stream from the reflux drum is recycled back into the reactor, after being compressed to 110 bar.

*Table 1. Key performance indicators for the Conventional Process.*

| Configuration | Conv | Unit |
|---|---|---|
| **MeOH production** | 102 | kt/y |
| **Recycle to feed ratio** | 4.6 | mol/mol |
| **Purge Fraction** | 0.022 | mol/mol |
| **$H_2$:CO ratio (reactor inlet)** | 5.9 | mol/mol |
| **$H_2$ conversion (per pass)** | 21.7 | % |
| **CO conversion (per pass)** | 46.1 | % |
| **Syngas use per unit of MeOH product** | 1.2 | kg/kg |

## 4.2 Processes Studied

Figures 6, 7 and 8 show the flowsheet of the processes, for both catalysts “A” and “B”. The stream summary for all configurations is situated Appendix C. In the simulation, compressor and pump efficiencies were set to the default 70%. Other block-specific characteristics are present in Appendix A.

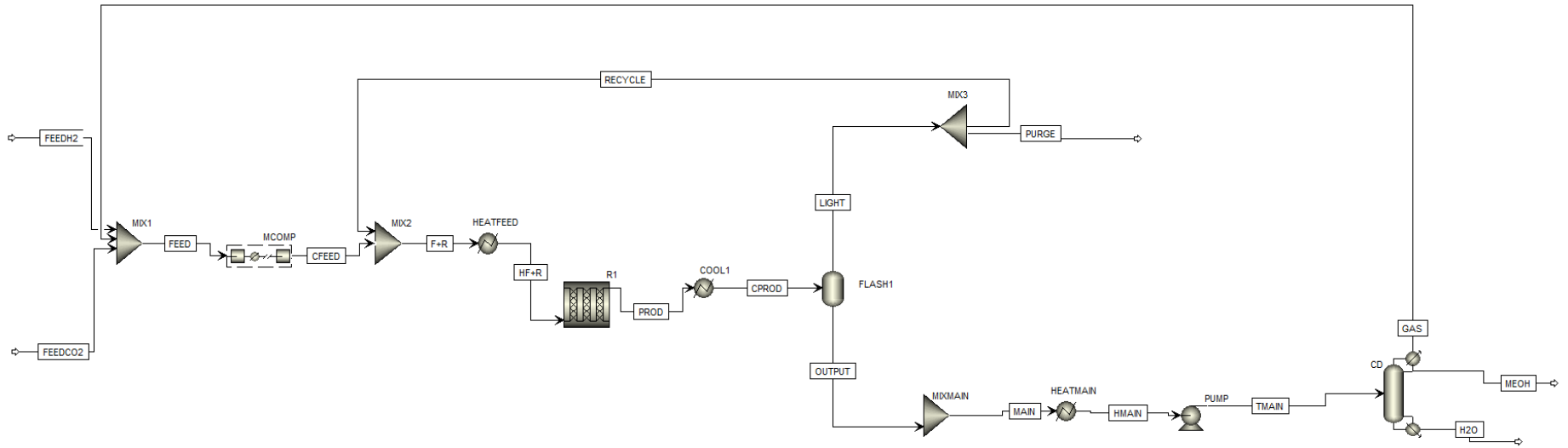



Figure 6. Process flowsheet for configuration I "Methanol Synthesis with a Recycle" for both catalysts.

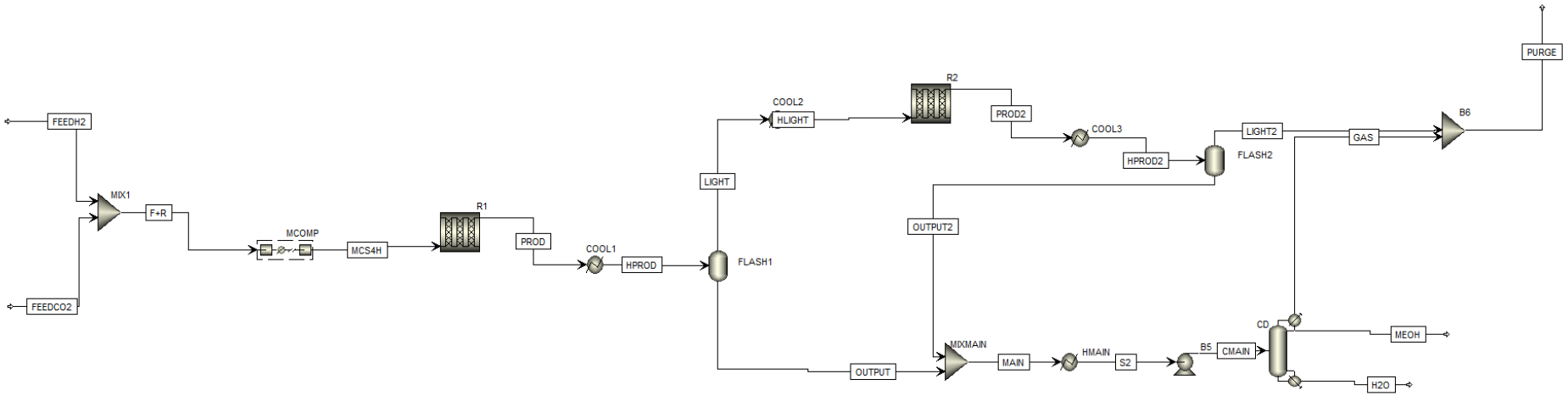



Figure 7. Process Flowsheet for Configuration II "Methanol Synthesis with Two Reactors in Series" for both catalysts.

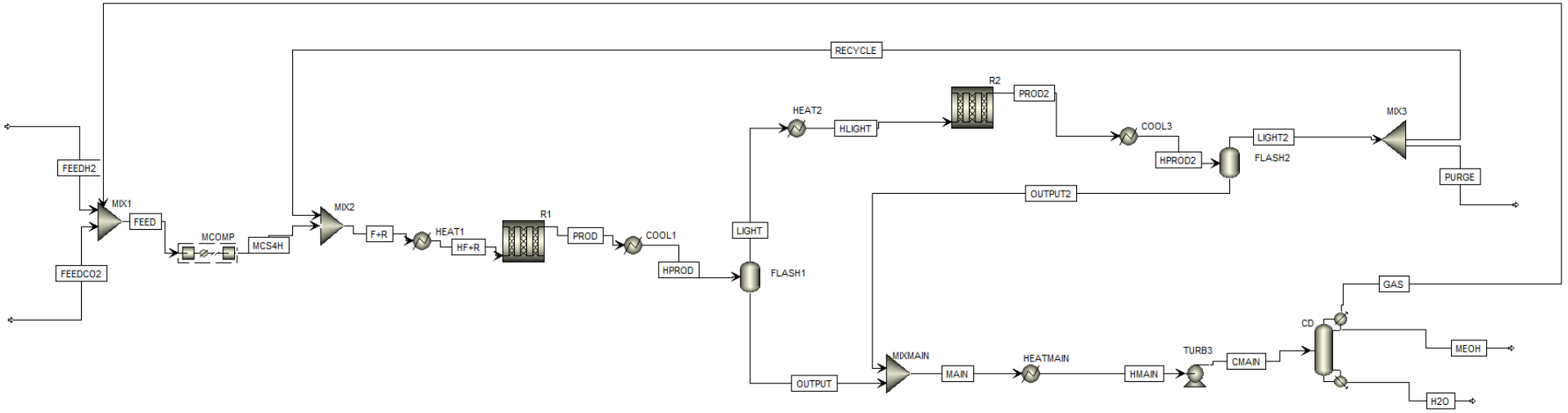



Figure 8. Process Flowsheet for Configuration III "Methanol Synthesis with Two Reactors in Series with a Recycle" for both catalysts.

### 4.2.1 Compression and Reactor Preheating

A hydrogen feed stream and carbon dioxide feed stream are mixed together at 1 bar, and then compressed in a four-stage compressor to 100 bar. Before the stream enters a reactor pre-heater, a recycled gas stream is added. A design spec of 6:1 was established for the ratio of hydrogen to carbon dioxide at the reactor inlet, varying the flow rate of each feed stream. This is necessary for an adequate simulation of the recycle stream in the process.

The feed stream with the added recycle stream then enters a heater at a design-specific temperature, exiting at a design-specific reactor temperature and pressure of 100 bar.

### 4.2.2 Reactor

The reactor specifications for every simulation are explicit in Appendix A, Table 15. The reactor kinetics are shown in Annex A. Sensitivity analyses for optimal temperature and pressure were carried, with the optimal operating conditions shown in Appendix A, Table 15. The reactor size was first tested utilizing the reactor residence time of approximately 13 seconds by Kiss et al. (2016), maintaining it as a constant for every simulation and varying the number of tubes in the reactor.

### 4.2.3 Flash Separator

After the reaction, the stream is cooled to 5 ºC. At this temperature, the separation in the Flash Separator occurs optimally, while still preventing the freezing of any stream component. The liquid effluent is then fed to the distillation part of the process.

In configuration I, designated by “Methanol Synthesis with a Recycle”, the gas effluent is subsequently purged at a fraction of 0.02. The rest of the effluent is fed back into the feed stream. Since the flash separator is operated at 100 bar, there is no need for further compressor work to get the recycle stream at the required pressure.

In configuration II, designated by “Methanol Synthesis with Two Reactors in Series”, the gas effluent is fed to a second reactor, being pre-heated to the optimized reactor temperature, and cooled afterwards to 5 ºC, before being fed to a second flash separator. The liquid effluent is, again, fed to the distillation part of the process, while the second gas effluent is completely purged.

In configuration III, designated by “Methanol Synthesis with Two Reactors in Series with a Recycle”, the gas effluent is fed similarly to configuration II. However, the second gas effluent, instead of being completely purged, is purged at a fraction of 0.02 and recycled back into the feed stream.

### 4.2.4 Distillation

Before being fed to the distillation column, the liquid effluent needs to be depressurized, while maintaining a 0.00% vapor fraction and a temperature above the freezing point for any of the components. The stream is heated from 5 ºC to a design-specific temperature, and depressurized to 5 bar. The stream then flows to a distillation column with a partial condenser operating at 0.8 bar, separating water as the bottom product, methanol as the high purity liquid distillate and a light gas distillate, which may be recycled to the feed stream. For all process configurations, molar methanol purity was specified for a minimum of 99.85%. The distillation column specifications for each simulation are explicit in Appendix A, Table 16.

*Table 2. Key performance indicators for all process configurations for methanol synthesis.*

| **Catalyst** | **A** | | | **B** | | | |
|---|---|---|---|---|---|---|---|
| **Configuration** | **I** | **II** | **III** | **I** | **II** | **III** | **Unit** |
| **MeOH production** | 101 | 101 | 100 | 99.0 | 100 | 101 | kt/y |
| **Recycle to feed ratio** | 2.4 | - | 1.2 | 0.76 | - | 0.73 | mol/mol |
| **Purge Fraction** | 0.02 | 1.0 | 0.02 | 0.02 | 1.0 | 0.02 | mol/mol |
| **$H_2$:$CO_2$ ratio (reactor inlet)** | 6.0 | 6.0 | 6.0 | 6.0 | 6.0 | 6.0 | mol/mol |
| **$H_2$ conversion (per pass)** | 24.5 | 38.7 | 39.2 | 49.1 | 49.8 | 49.8 | % |
| **$CO_2$ conversion (per pass)** | 49.2 | 80.6 | 79.8 | 98.5 | 100 | 100 | % |
| **$CO_2$ use per unit of MeOH product** | 1.40 | 1.80 | 1.38 | 1.38 | 1.38 | 1.38 | kg/kg |
| **$H_2$ use per unit of MeOH product** | 0.20 | 0.50 | 0.20 | 0.19 | 0.38 | 0.19 | kg/kg |

## 4.3 Heat Integration

The heat integration for all designs and simulations was completed utilizing the software *Aspen Energy Analyzer*, specifying a minimum temperature approach of 10 ºC.

Medium-pressure steam generation was used in order to cool down the reactors for each configuration. However, configurations II and III for catalyst "B" utilize Low-pressure steam generation as well, since the second reactor functions at a lower temperature. Refrigerant at -25 ºC was used to cool the reactor output to 5 ºC.

The heat integration process was focused on minimizing utility usage. It is possible, for the economic analysis, that further optimizations can be made, regarding utility usage versus heat exchanger area.

*Table 3. Utility usage for each simulation.*

| Catalyst | A | | | B | | | Conv | Unit |
|---|---|---|---|---|---|---|---|---|
| Configuration | I | II | III | I | II | III | | |
| Electricity | 9.23 | 19.11 | 8.92 | 8.70 | 14.55 | 10.16 | 8.65 | MW |
| Cooling Water | 19.47 | 25.61 | 19.72 | 17.91 | 21.79 | 18.94 | 19.29 | |
| LP Steam Generation | - | - | - | - | 0.61 | 0.76 | - | |
| MP Steam Generation | 6.72 | 6.54 | 6.66 | 6.77 | 6.18 | 6.09 | - | |
| HP Steam Generation | - | - | - | - | - | - | 6.54 | |
| Refrigerant | 2.10 | 1.64 | 1.31 | 0.39 | 0.53 | 0.53 | - | |
| Hot Oil | 5.26 | 0.55 | 3.87 | 2.63 | 0.24 | 3.77 | - | |

Heat exchanger networks for every simulation are explicit in Appendix D.

## 4.4 Economic Evaluation

The economic analysis for all designs and simulations was based on the equipment purchase costs, obtained by the *Aspen Process Economic Analyzer* function, integrated in the *Aspen Plus* software. For certain process blocks, such as reactors and multi-stage compressors, an online cost estimation tool, accompanying Plant Design and Economics for Chemical Engineers, 5th edition, Peters, Timmerhaus, and West, was used. For the overall cost estimation for each design, the spreadsheet "Cost and Evaluation Workbook", accompanying Plant Design and Economics for Chemical Engineers, 5th edition, Peters, Timmerhaus, and West was utilized, along with correlations provided in a support book by Martins (2018), both present in Annex C.

### 4.4.1 Simulation Comparison

Table 4 compares the different economic indicators for each process configuration. A depreciation of 10 years was considered, along with a yearly inflation rate of 0.0225 (Portugal Inflation Rate, 2021), a minimum acceptable rate of return of 1% and an income tax rate of 0.35. For the first year, a 50% operation rate was assumed, and for the second year, a 90% operation rate.

*Table 4. Economic Analysis for all process configurations for methanol synthesis, with a 25% uncertainty in equipment purchase cost, for a 100 kt/y methanol plant.*

| **Catalyst** | **A** | | | **B** | | | **Conv** | **Unit** |
|---|---|---|---|---|---|---|---|---|
| **Configuration** | **I** | **II** | **III** | **I** | **II** | **III** | | |
| **Total capital investment** | 17.91 ± 4.48 | 32.91 ± 8.23 | 19.58 ± 4.89 | 17.42 ± 4.35 | 33.04 ± 8.26 | 19.13 ± 4.78 | 30.21 ± 7.55 | M€ |
| **Total production cost** | 37.80 ± 0.38 | 91.42 ± 0.65 | 37.39 ± 0.39 | 35.19 ± 0.37 | 70.32 ± 0.65 | 36.57 ± 0.38 | 39.43 ± 0.77 | M€/y |
| **Cost per ton of MeOH product** | 375.2 ± 3.8 | 908.2 ± 6.4 | 373.3 ± 3.9 | 355.5 ± 3.8 | 701.5 ± 6.5 | 362.1 ± 3.7 | 393.7 ± 7.7 | €/t |
| **Return on investment** | 6.38 | -174 | 5.91 | 14.7 | -106 | 10.7 | -2.03 | %/y |
| **Return period** | 5.72 | -0.49 | 5.92 | 3.62 | -0.83 | 4.41 | 13.9 | y |

Firstly, it can easily be concluded that configuration II is not economically feasible for both catalysts. The lack of a recycle stream, which means a complete purge of unreacted components, forces an increase in raw material purchase for the same amount of methanol produced. The almost thrice-fold increase in hydrogen feed usage is damning for the overall production cost for this configuration.

An important optimization is the use of a multi-stage compressor in the feed stream only, maintaining the main process pressure at 100 bar. This allows for a minimum use of electricity for compression.

Despite the differences in total capital investment and total production cost, configurations I and III present similar results for the cost per ton of synthesized methanol. This is due to the variation in total capital investment being offset by a small variation in raw material consumption.

Comparing the different catalysts “A” and “B”, there is a significant difference between production costs per ton of synthesized methanol, due to a respective increase in raw material conversion to methanol.

Interestingly, whereas with catalyst “A” both configurations, I and III, are similar in terms of production cost, with catalyst “B” there is a noticeable difference between the two. Due to catalyst “B” providing a very high conversion in just one reactor, the second reactor in

configuration III does not bring enough value to compensate for the added equipment cost of a second reactor and flash separator.

It would seem that in order to maximize profits, the usage of fossil hydrogen feedstock and green sourced carbon dioxide is paramount. However, section 4.4.3 studies the usage of completely fossil and completely green feedstock.

### 4.4.2 Sensitivity analysis of the methanol production cost

Figure 9 shows the impacts of the raw materials cost and CAPEX in the overall methanol production cost, with a variation of 25% for each parameter value.

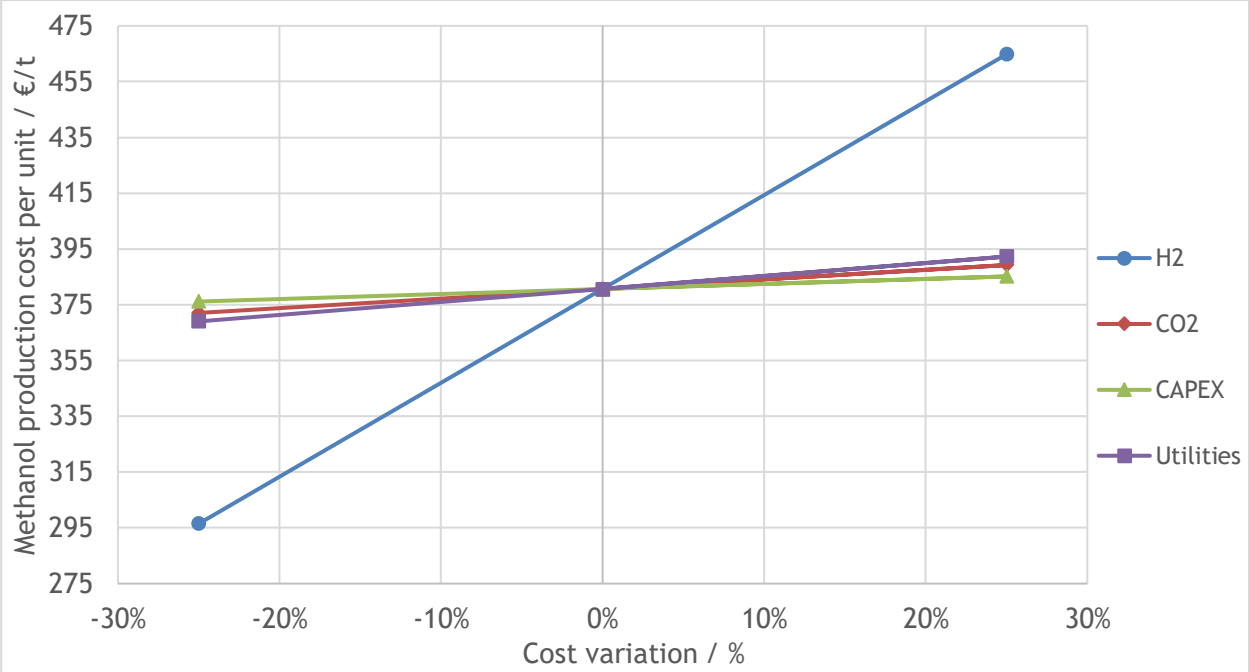



*Figure 9. Impacts on methanol production cost for feedstocks, capital expenditures and utilities.*

In the case of the hydrogen price impact, the results show a significant impact on methanol production costs – a variation of 25% in the price of hydrogen results in a variation of approximately 22% for the average methanol production cost.

In terms of carbon dioxide price impact, a price variation slightly impacts the average methanol production cost. A variation of 25% in carbon dioxide prices results in approximately 2% variation for the methanol production cost. This occurs due to two factors: first, for the same amount, the cost of hydrogen is two orders of magnitude greater compared to the cost of carbon dioxide; second, the amount of molar hydrogen in the process feed stream is consumed at a three times higher rate than the amount of molar carbon dioxide in the process feed stream.

In the case of the impact of CAPEX in the overall methanol production cost, there is also only a slight impact. A variation of 25% in the overall CAPEX only impacts the methanol production

cost by approximately 1%. In terms of utility costs, a variation of 25% impacts methanol synthesis costs by approximately 3%.

These results show that for these designs, the overall methanol production cost is dictated primarily by the cost of hydrogen. As such, it can be concluded that a further optimization of the operating conditions or utility usage can possibly offset an increase in carbon dioxide price, but will not offset an increase in hydrogen price.

### 4.4.3 Green Methanol versus Fossil Methanol

Table 5 shows the impact of fossil versus green raw material prices in the overall methanol production cost using catalyst "A", for the years of 2021 and 2025.

*Table 5. Fossil versus green methanol prices, for the years of 2021 and 2025, utilizing catalyst "A".*

| Year | 2021 | 2025 | 2021 | 2025 | 2021 | 2025 | Unit |
|---|---|---|---|---|---|---|---|
| $H_2$ | 1.50 | 1.94 | 2.45 | 2.45 | 3.16 | 3.16 | €/kg |
| $CO_2$ (allowances) | 0.06 | 0.10 | - | - | - | - | €/kg |
| $CO_2$ (emissions avoided) | - | - | -0.03 | -0.07 | -0.03 | -0.07 | €/kg |
| TPC | 50.7 | 68.1 | 57.9 | 51.6 | 75.0 | 68.7 | M€/year |
| Electricity price | 45.0 | 60.0 | 45.0 | 45.0 | 60.0 | 60.0 | €/MWh |
| TPC/t MeOH | 507 | 681 | 579 | 516 | 750 | 687 | €/t MeOH |
| TPC/t MeOH, without $CO_2$ | 413 | 524 | - | - | - | - | €/t MeOH |

The cost of carbon dioxide for 2021 and 2025 is, respectively, 60 €/t and 100 €/t. Concerning green carbon dioxide, the price was calculated by subtracting, from a purification cost of 30 €/t, the cost of purchased carbon dioxide.

For the price of fossil hydrogen, the values 1.5 €/kg and 1.94 €/kg were utilized for the years 2021 and 2025, respectively. In the case of green hydrogen price, the calculations are made for two different values, respectively 2.45 €/kg and 3.16 €/kg, for both 2021 and 2025 (Mendes, 2021).

Calculations were also made for the production of Methanol without the cost of carbon dioxide, resulting in a production cost per unit of methanol of 413 €/t for 2021, which compares nicely with the Methanex European Posted Contract Price of 410 €/t, valid from July 1, 2021 to September 30, 2021.

For 2021, fossil methanol has a more competitive production cost than green methanol by approximately 14%, with a difference of 72 €/t.

For 2025, at a green hydrogen price of 2.45 €, green methanol production becomes quite competitive with the 2021 fossil methanol production costs, with discrepancy of about 2%. The 2025 fossil methanol production cost is competitive only to the worst-case-scenario green methanol production costs, with an increase from the former to the latter of approximately 1%.

*Table 6. Fossil versus green methanol prices, for the years of 2021 and 2025, utilizing catalyst "B".*

| Year | 2021 | 2025 | 2021 | 2025 | 2021 | 2025 | Unit |
|---|---|---|---|---|---|---|---|
| **H2** | 1.50 | 1.94 | 2.45 | 2.45 | 3.16 | 3.16 | €/kg |
| **CO2 (allowances)** | 0.06 | 0.10 | - | - | - | - | €/kg |
| **$CO_2$ (emissions avoided)** | - | - | -0.03 | -0.07 | -0.03 | -0.07 | €/kg |
| **TPC** | 47.2 | 62.6 | 54.5 | 48.4 | 68.8 | 63.9 | M€/year |
| **Electricity price** | 45.0 | 60.0 | 45.0 | 45.0 | 60.0 | 60.0 | €/MWh |
| **TPC/t MeOH** | 476 | 632 | 545 | 484 | 688 | 639 | €/t MeOH |
| **TPC/t MeOH, without $CO_2$** | 385 | 491 | - | - | - | - | €/t MeOH |

Comparing the results for catalyst "A" with the same calculations for catalyst "B", the average decrease in production cost per unit of methanol produced is of approximately 6%, which translates to an average cost reduction of 37 €/t.

# 5 Conclusion

This work compares three different process configurations of methanol synthesis via direct carbon dioxide hydrogenation for two different catalysts, and the conventional process comprehending natural gas reforming followed by methanol synthesis, for a total of seven simulations. The three process configurations were optimized for minimum methanol production cost, featuring methanol production with a recycle, methanol production with two reactors in series and methanol production with two reactors in series with a recycle.

The methanol production costs were compared across all configurations, showing that methanol production with two reactors in series – process configuration II – is not economically feasible, due to the purge of a large current of unreacted products. Process configurations I and III, showed the most economically competitive results; however, going from catalyst "A" to catalyst "B" showed a dramatic increase in conversion rates. As such, catalyst "B" shows that configuration I has the *de facto* lowest methanol production cost of all configurations, due to configuration III having an unnecessary second reactor.

An economic analysis of the feedstock price impacts on the production of the green methanol shows that hydrogen feedstock has the highest impact, accounting for *ca*. 80% of the cost structure of the green methanol; on the other hand, $CO_2$ has a humble contribution for the green methanol cost structure of just 8%. A comparison between fossil methanol synthesis and green methanol synthesis indicated that by 2025, green methanol should become price competitive, which allows for a unique economic opportunity.

# 6 Assessment of the work done

## 6.1 Objectives Achieved

For this thesis, the design and simulation of methanol synthesis through carbon dioxide hydrogenation, not only for different process configurations, but also for two different catalysts - a highly active Cu/Zn/Al/Zr fibrous catalyst and an experimental catalyst – was completed successfully: it was possible to see which configurations were efficient in the production of methanol. Also, a simulation of the conventional process of methanol synthesis from synthetic gas was made, which allowed for a comparison to be drawn between all simulations.

The economic analysis for each design was successful, showing an accurate description and assessment of methanol production costs, with the conventional process working as a sort of "control". The measurement of the impact of different process variables in the methanol production cost was also carried out correctly.

Finally, the economic analysis of fossil versus green methanol was also carried out successfully, with the fossil methanol production cost without $CO_2$ giving a very accurate value compared to the current prices, provided by Methanex (2021).

## 6.2 Other Work Carried Out

A simulation was made to verify the work of Kiss et al. (2016), in order to confirm that an accurate implementation of the reaction kinetics was made by the author of the current work.

## 6.3 Final Assessment

In the opinion of the author, this work acts as a culmination of most recent green methanol studies: not only does it serve as an in-depth guide for cost-efficient methanol synthesis, but also as an innovative set piece in worldwide methanol synthesis, with an exhaustive study of the impact a bifunctional catalyst has on the processes studied. On top of this, this work also presents a reasonably accurate prediction of methanol synthesis costs in the near-future.

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# Annex A - Catalyst kinetics by Kiss et al. (2013)

*Table 7. Kinetic factor for reactions A, B and C.*

| Reaction | k | n | $E_a$ [J/mol.K] |
|---|---|---|---|
| A | $4.0638 \cdot 10^{-6}$ [kmol./$kg_{cat}$.s.Pa] | 0 | 11695 |
| B | $9.0421 \cdot 10^{8}$ [kmol/$kg_{cat}$.s.$Pa^{1/2}$] | 0 | 112860 |
| C | $1.5188 \cdot 10^{-33}$ [kmol/$kg_{cat}$.s.Pa] | 0 | 266010 |

*Table 8. Constants for driving force, using the format for Aspen Plus.*

| | $K_1$ | | $K_2$ | |
|---|---|---|---|---|
| **Reaction** | **A** | **B** | **A** | **B** |
| A | -23.20 | 14225 | 28.895 | 2385 |
| B | -22.48 | 9777 | -28.12 | 15062 |
| C | -22.48 | 9777 | 23.974 | 3222 |

*Table 9. $K_i$ factors for the adsorption term, using the format for Aspen Plus.*

| Term | Expression | $A_i=\ln(a_i)$ | $B_i=b_i/R$ | $\prod c_j^{\nu_j}$ |
|---|---|---|---|---|
| 1 | 1 | 0 | 0 | $\sqrt{f_{H_2}}$ |
| 2 | $\frac{K_{H_2O}}{\sqrt{K_H}}$ | -26.1568 | 13842 | $f_{H_2O}$ |
| 3 | $K_{CO}$ | -23.2006 | 14225 | $f_{CO}\sqrt{f_{H_2}}$ |
| 4 | $\frac{K_{CO}K_{H_2O}}{\sqrt{K_H}}$ | -49.3574 | 28067 | $f_{CO}f_{H_2O}$ |
| 5 | $K_{CO_2}$ | -22.4827 | 9777 | $f_{CO_2}\sqrt{f_{H_2}}$ |
| 6 | $\frac{K_{CO_2}K_{H_2O}}{\sqrt{K_H}}$ | -48.6395 | 23619 | $f_{CO_2}f_{H_2O}$ |

# Annex B - Catalyst kinetics used the Conventional Process

*Table 10. Catalyst kinetics used by Luyben (2010)*

| $R_1$ ($CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$) | |
|---|---|
| kinetic factor | $k = 1.07 \times 10^{-3}$<br>$E = 36\,696$ kJ/kmol |
| driving-force expressions | |
| term 1 | |
| conc. exponents for reactants: | $CO_2 = 1$; $H_2 = 1$ |
| conc. exponents for products: | $CH_3OH = 0$; $H_2O = 0$ |
| coefficients: | $A = -23.02581$; $B = C = D = 0$ |
| term 2 | |
| conc. exponents for reactants: | $CO_2 = 0$; $H_2 = -2$ |
| conc. exponents for products: | $CH_3OH = 1$; $H_2O = 1$ |
| coefficients: | $A = 24.388981$; $B = -7059.7258$;<br>$C = D = 0$ |
| adsorption expression | |
| adsorption term exponent: | 3 |
| concentration exponents: | |
| term 1: | $H_2 = 0$; $H_2O = 0$ |
| term 2: | $H_2 = -1$; $H_2O = 1$ |
| adsorption constants: | |
| term 1: | $A = 0$, $B = 0$, $C = 0$, $D = 0$ |
| term 2: | $A = 8.1471087$, $B = 0$, $C = 0$, $D = 0$ |
| $R_2$ ($CO_2 + H_2 \rightarrow CO + H_2O$) | |
| kinetic factor | $k = 1.22 \times 10^{9}$<br>$E = 94765$ kJ/kmol |
| driving-force expressions | |
| term 1 | |
| conc. exponents for reactants: | $CO_2 = 1$; $H_2 = 0$ |
| conc. exponents for products: | $CO = 0$; $H_2O = 0$ |
| coefficients: | $A = -11.512952$; $B = C = D = 0$ |
| term 2 | |
| conc. exponents for reactants: | $CO_2 = 0$; $H_2 = -1$ |
| conc. exponents for products: | $CO = 1$; $H_2O = 1$ |
| coefficients: | $A = -16.184871$; $B = 4773.2589$;<br>$C = D = 0$ |
| adsorption expression | |
| adsorption term exponent: | 1 |
| concentration exponents: | |
| term 1: | $H_2 = 0$; $H_2O = 0$ |
| term 2: | $H_2 = -1$; $H_2O = 1$ |
| adsorption constants: | |
| term 1: | $A = 0$, $B = 0$, $C = 0$, $D = 0$ |
| term 2: | $A = 8.1471087$, $B = 0$, $C = 0$, $D = 0$ |

# Annex C - Economic Analysis Spreadsheet by Peters, Timmerhaus and West

*Table 11. Example of a Capital Investment page, with correlations sourced from a book by Martins (2018).*

| **Project Identifier: Methanol Synthesis (example)** | **User: copy from values at left or insert** | **Calculated values, million €** |
|---|---|---|
| **Direct Costs** | | |
| **Purchased equipment, E'** | | **8.800** |
| **Delivery, fraction of E'** | 0.10 | 0.880 |
| **Subtotal: delivered equipment** | | 9.680 |
| **Purchased equipment installation** | 0.10 | 0.968 |
| **Instrumentation&Controls(installed)** | 0.05 | 0.484 |
| **Piping (installed)** | 0.12 | 1.113 |
| **Electrical systems (installed)** | 0.06 | 0.581 |
| **Buildings (including services)** | 0.11 | 1.016 |
| **Yard improvements** | 0.04 | 0.339 |
| **Service facilities (installed)** | 0.14 | 1.355 |
| **Total direct costs** | 0.61 | 15.536 |
| **Indirect Costs** | | |
| **Engineering and supervision** | 0.13 | 1.210 |
| **Construction expenses** | 0.10 | 0.968 |
| **Legal expenses** | 0.04 | 0.387 |
| **Contractor's fee** | 0.04 | 0.387 |
| **Contingency** | 0.10 | 0.968 |
| **Total indirect costs** | 0.41 | 3.920 |
| **Fixed capital investment (FCI)** | | **19.457** |
| **Working capital (WC)** | 0.45 | **4.390** |
| **Total capital investment (TCI)** | | **23.847** |

*Table 12. Annual Operating Labour Costs, localized for Portugal, EUROSTAT (2021).*

| Operating Labor | | | |
|---|---|---|---|
| **Number of operators per shift*** | **Shifts per day**** | **Operator rate, €/h** | **Annual operating labor cost, million €/y** |
| 5 | 3 | 12.8 | **0.561** |

*Table 13. Example of an Utility Costs page, with unit costs for every utility used. Prices from Aspen Energy Analyzer and Martins (2018).*

| **TOTAL UTILITY COST =** | | **-** | **million €/y** | | |
|---|---|---|---|---|---|
| **Utility** | **Default unit cost** | **Default cost units** | **Annual utility requirement,** | **Default units of utility requirement** | **Annual utility cost, million €/y** |
| **Electricity** | | | | | |
| Purchased, average | 0.050 | €/kWh | - | kWh/y | - |
| Hot oil | 2.79 | €/GJ | - | GJ/y | - |
| **Cooling Water** | 0.04 | €/GJ | - | GJ/y | - |
| Refrigeration, to temperature | | | | | |
| -25 °C | 6.37 | €/GJ | - | GJ/y | - |
| **HP Steam Generation** | -1.98 | €/GJ | - | GJ/y | - |
| Waste water | | | | | |
| Treatment (kg removed) | 0.29 | €/kg | - | kg/y | - |
| **LP Steam Generation** | -1.50 | €/GJ | - | GJ/y | - |
| MP Steam Generation | -1.74 | €/GJ | - | GJ/y | - |

*Table 14. Example of an Annual Total Product Cost page, with correlations sourced from a book by Martins, 2018.*

| **Capacity** | 100 | **$10^6$ kg per year** | | |
|---|---|---|---|---|
| **Fixed Capital Investment, FCI** | 19.457 | **million €** | | |
| **Item** | **Default factor, user may change** | **Basis** | **Basis cost, million €/y** | **Cost, million €/y** |
| **Raw materials** | | | | 12.650 |
| **Operating labor** | | | | 0.885 |
| **Operating supervision** | 0.15 | of operating labor | 0.885 | 0.133 |
| **Utilities** | | | | 3.114 |
| **Maintenance and repairs** | 0.03 | of FCI | 19.457 | 0.584 |
| **Operating supplies** | 0.0075 | of maintenance & repair | 0.584 | 0.004 |
| **Laboratory charges** | 0.15 | of operating labor | 0.885 | 0.133 |
| **Royalties (if not on lump-sum basis)** | 0.01 | of $c_o$ | 21.911 | 0.219 |
| **Catalysts and solvents** | 0.001 | of FCI | 19.457 | 0.019 |
| **Variable cost =** | | | | **17.741** |
| **Taxes (property)** | 0.02 | of FCI | 19.457 | 0.389 |
| **Financing (interest)** | 0 | of FCI | 19.457 | 0.000 |
| **Insurance** | 0.007 | of FCI | 19.457 | 0.136 |
| **Rent** | 0.02 | of FCI | 19.457 | 0.389 |
| **Depreciation** | Calculated separately | | | |
| **Fixed Charges =** | | | | **0.914** |
| **Plant overhead, general** | 0.6 | of labor, supervision and maintenance | 1.601 | 0.961 |
| **Plant Overhead =** | | | | **0.961** |
| **Manufacturing cost =** | | | | **19.616** |
| **Administration** | 0.2 | of labor, supervision and maintenance | 1.601 | 0.320 |
| **Distribution & selling** | 0.05 | of $c_o$ | 21.911 | 1.096 |
| **Research & Development** | 0.04 | of $c_o$ | 21.911 | 0.876 |
| **General Expense =** | | | | **2.292** |
| **TOTAL PRODUCT COST WITHOUT DEPRECIATION = $c_o$ =** | | | | **21.911** |

# Appendix A – Block Characteristics

*Table 15. Reactor Characteristics for each simulation*

| Catalyst | A | | | | | B | | | | | Conv | Unit |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Configuration | I | II | | III | | I | II | | III | | | |
| Reactor | 1 | 1 | 2 | 1 | 2 | 1 | 1 | 2 | 1 | 2 | 1 | - |
| Tubes | 403 | 261 | 192 | 252 | 185 | 154 | 161 | 80 | 163 | 87 | 1710 | - |
| Length | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 10.5 | 12.2 | m |
| Diameter | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.05 | 0.03675 | m |
| Catalyst Loading | 318.7 | 204.9 | 120.3 | 198.0 | 118.7 | 318.7 | 204.9 | 120.3 | 198.0 | 118.7 | - | kg |
| Bed voidage | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.98 | 0.5 | - |
| Temperature | 255 | 255 | 255 | 255 | 255 | 232 | 234 | 150 | 240 | 180 | 272 | ºC |
| Pressure | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 107 | bar |

*Table 16. Distillation Column characteristics for each simulation*

| Catalyst | A | | | B | | | Conv | Unit |
|---|---|---|---|---|---|---|---|---|
| Configuration | I | II | III | I | II | III | | |
| Stages | 30 | 30 | 30 | 30 | 30 | 30 | 42 | - |
| Feed | 22 | 20 | 20 | 20 | 22 | 22 | 27 | - |
| Reflux Ratio | 2 | 2 | 2 | 2 | 2 | 2.5 | 1 | kg/kg |
| Distillate to Feed fraction | 0.5074 | 0.4952 | 0.5062 | 0.5011 | 0.5002 | 0.5005 | 0.8325 | - |
| Distillate Vapor fraction | 0.04 | 0.029 | 0.032 | 0.005 | 0.0025 | 0.0025 | - | - |
| Pressure | 0.8 | 0.8 | 0.8 | 0.8 | 0.8 | 0.8 | 1 | bar |

# Appendix B – Utility and Component Prices

*Table 17. Utility temperatures and cost per unit of energy*

| | | Temperature, inlet / °C | Temperature, outlet / °C | Cost / €/GJ |
|---|---|---|---|---|
| **Refrigerant** | | -25 | -24 | 6.368 |
| **Cooling Water** | | 20 | 30 | 0.0399 |
| **LP Steam Generation** | | 124 | 125 | - 1.504 |
| **MP Steam Generation** | | 174 | 175 | -1.743 |
| **HP Steam Generation** | | 249 | 250 | -1.982 |
| **Hot Oil** | **Configuration I, Catalyst "A"** | 280 | 250 | 2.786 |
| | **Catalyst "A"** | 290 | 260 | |
| | **Catalyst "B"** | 300 | 270 | |

*Table 18. Costs utilized for other utilities, raw materials and products.*

| | Cost | Unit |
|---|---|---|
| **Wastewater treatment** | 0.29 | €/kg organics removed |
| **Electricity** | 0.50 | €/kWh |
| **Methanol** | 0.41 | €/kg |
| **H2** | 1.50 | €/kg |
| **CO2** | -0.022 | €/kg |

# Appendix C – Stream Summary

*Table 19. Stream Summary for the Conventional Process.*

| | Units | 1 | 4 | 5 | 7 | 8 | 9 | 10 | 12 | 13 | 14 | 16 | 17 | 18 | 20 | 22 | 23 | 24 | 26 | 27 | MCS4 | METHANC | WATER |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | | | | | |
| From | | | B6 | B20 | B15 | B16 | B21 | B11 | R1 | B7 | B11 | B21 | B14 | B10 | B9 | B10 | B4 | B12 | B3 | B8 | B1 | B8 | B8 |
| To | | B1 | R1 | B16 | B16 | B6 | B11 | | B7 | B21 | B12 | B14 | B10 | B9 | B8 | B4 | B20 | B20 | B15 | B3 | B15 | | |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | | | | | | | | | | | | | | | | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | | | | | |
| Phase | | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Phase | | Vapor Pha | Liquid Phase | | Liquid Phase | | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Vapor Pha | Liquid Pha | Liquid Pha |
| Temperature | C | 50 | 150 | 46.29332 | 194.2062 | 72.98127 | 38 | 38 | 272.25 | 38 | 38 | 38 | 34.4062 | 38 | 37.14847 | 38 | 507.8254 | 41.67635 | 542.4306 | 50 | 189.5563 | 50 | 99.52757 |
| Pressure | bar | 1 | 110 | 110 | 110 | 110 | 106.5 | 106.5 | 107.3032 | 107.3032 | 106.5 | 106.5 | 2 | 2 | 1 | 2 | 110 | 110 | 110 | 1 | 110 | 1 | 1 |
| Molar Vapor Fraction | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.914097 | 1 | 0 | 0.068334 | 0 | 0.005658 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 |
| Molar Liquid Fraction | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.085903 | 0 | 1 | 0.931666 | 1 | 0.994342 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 |
| Molar Solid Fraction | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Mass Vapor Fraction | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.816987 | 1 | 0 | 0.082837 | 0 | 0.007558 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 |
| Mass Liquid Fraction | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.183013 | 0 | 1 | 0.917163 | 1 | 0.992442 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 |
| Mass Solid Fraction | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Molar Enthalpy | kcal/mol | -13.0375 | -15.3614 | -16.9083 | -12.3472 | -16.0015 | -16.591 | -16.591 | -17.5506 | -20.3717 | -16.591 | -60.6199 | -60.6199 | -59.5581 | -59.5581 | -72.9075 | -67.6733 | -16.5624 | -61.2122 | -67.5718 | -12.0059 | -56.3837 | -66.8876 |
| Mass Enthalpy | kcal/kg | -1146.4 | -1218.75 | -1314.24 | -1068.9 | -1269.54 | -1305.98 | -1305.98 | -1234.86 | -1433.36 | -1305.98 | -2002.21 | -2002.21 | -1998.95 | -1998.95 | -1992.81 | -1849.74 | -1303.73 | -1647.89 | -1819.09 | -1055.7 | -1759.61 | -3710.98 |
| Molar Entropy | cal/mol-K | 6.867948 | -6.21862 | -10.1144 | 0.06207 | -7.88817 | -10.2555 | -10.2555 | -6.85201 | -13.8474 | -10.2555 | -51.9035 | -51.2991 | -54.4324 | -54.4253 | -5.04131 | -3.02204 | -10.2301 | -12.5436 | -14.8798 | 0.074588 | -55.6277 | -34.8974 |
| Mass Entropy | cal/gm-K | 0.603907 | -0.49338 | -0.78617 | 0.005373 | -0.62584 | -0.80727 | -0.80727 | -0.48211 | -0.9743 | -0.80727 | -1.71432 | -1.69436 | -1.82692 | -1.82668 | -0.1378 | -0.0826 | -0.80527 | -0.33769 | -0.40058 | 0.006559 | -1.73602 | -1.93614 |
| Molar Density | kmol/cum | 0.037203 | 2.987953 | 4.042205 | 2.691204 | 3.681754 | 4.02993 | 4.02993 | 2.280875 | 4.359723 | 4.02993 | 20.56359 | 1.097793 | 20.27696 | 5.157842 | 0.078091 | 1.641638 | 4.102709 | 1.59129 | 0.037569 | 2.716682 | 23.79593 | 50.95691 |
| Mass Density | kg/cum | 0.423094 | 37.66074 | 52.00487 | 31.08686 | 46.40554 | 51.19572 | 51.19572 | 32.41708 | 61.96283 | 51.19572 | 622.5922 | 33.23726 | 604.1454 | 153.6762 | 2.856999 | 60.05989 | 52.12029 | 59.10991 | 1.395535 | 30.89552 | 762.4991 | 918.4602 |
| Enthalpy Flow | Gcal/hr | -17.7535 | -105.948 | -93.4325 | -16.931 | -110.364 | -93.1069 | -2.04835 | -107.742 | -125.061 | -91.0585 | -31.9503 | -31.9503 | -29.1637 | -29.1637 | -2.72615 | -2.53044 | -90.9021 | -0.58219 | -0.64267 | -16.3488 | -22.4494 | -5.48492 |
| Average MW | | 11.37252 | 12.60419 | 12.86547 | 11.55128 | 12.60419 | 12.70387 | 12.70387 | 14.21256 | 14.21256 | 12.70387 | 30.27643 | 30.27643 | 29.79468 | 29.79468 | 36.58533 | 36.58533 | 12.70387 | 37.14591 | 37.14591 | 11.37252 | 32.04325 | 18.02425 |
| Mole Flows | kmol/hr | 1361.731 | 6897.079 | 5525.837 | 1371.242 | 6897.079 | 5611.907 | 123.4619 | 6138.966 | 6138.966 | 5488.445 | 527.0596 | 527.0596 | 489.6676 | 489.6676 | 37.39191 | 37.39191 | 5488.445 | 9.510953 | 9.510953 | 1361.731 | 398.1547 | 82.00198 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | | | | | |
| H2 | | 0.672083 | 0.565774 | 0.540549 | 0.667423 | 0.565774 | 0.543997 | 0.543997 | 0.497502 | 0.497502 | 0.543997 | 0.002444 | 0.002444 | 2.57E-06 | 2.57E-06 | 0.034423 | 0.034423 | 0.543997 | 0.000132 | 0.000132 | 0.672083 | 1.73E-09 | 1.00E-33 |
| CO2 | | 0.07063 | 0.105341 | 0.113328 | 0.073156 | 0.105341 | 0.109506 | 0.109506 | 0.104895 | 0.104895 | 0.109506 | 0.055796 | 0.055796 | 0.008569 | 0.008569 | 0.674263 | 0.674263 | 0.109506 | 0.434856 | 0.434856 | 0.07063 | 0.000151 | 1.83E-27 |
| CO | | 0.229073 | 0.095667 | 0.062956 | 0.227485 | 0.095667 | 0.063334 | 0.063334 | 0.057942 | 0.057942 | 0.063334 | 0.00053 | 0.00053 | 1.14E-06 | 1.14E-06 | 0.007455 | 0.007455 | 0.063334 | 5.86E-05 | 5.86E-05 | 0.229073 | 7.61E-10 | 8.65E-27 |
| CH4 | | 0.023168 | 0.200258 | 0.244232 | 0.023049 | 0.200258 | 0.244953 | 0.244953 | 0.224775 | 0.224775 | 0.244953 | 0.009936 | 0.009936 | 0.000117 | 0.000117 | 0.138527 | 0.138527 | 0.244953 | 0.006001 | 0.006001 | 0.023168 | 1.05E-07 | 0 |
| H2O | | 0.002018 | 0.000952 | 0.000691 | 0.002004 | 0.000952 | 0.000583 | 0.000583 | 0.013986 | 0.013986 | 0.000583 | 0.156697 | 0.156697 | 0.167399 | 0.167399 | 0.016548 | 0.016548 | 0.000583 | 1.03E-05 | 1.03E-05 | 0.002018 | 5.07E-05 | 0.99936 |
| N2 | | 0.003027 | 0.026687 | 0.032563 | 0.003007 | 0.026687 | 0.032761 | 0.032761 | 0.02997 | 0.02997 | 0.032761 | 0.000248 | 0.000248 | 4.77E-07 | 4.77E-07 | 0.00349 | 0.00349 | 0.032761 | 2.46E-05 | 2.46E-05 | 0.003027 | 2.24E-10 | 3.26E-23 |
| CH3OH | | 0 | 0.005322 | 0.00568 | 0.003877 | 0.005322 | 0.004865 | 0.004865 | 0.070929 | 0.070929 | 0.004865 | 0.774348 | 0.774348 | 0.823911 | 0.823911 | 0.125296 | 0.125296 | 0.004865 | 0.558918 | 0.558918 | 0 | 0.999798 | 0.00064 |
| Mass Flows | kg/hr | 15486.31 | 86932.1 | 71092.5 | 15839.61 | 86932.1 | 71292.95 | 1568.445 | 87250.43 | 87250.43 | 69724.5 | 15957.48 | 15957.48 | 14589.49 | 14589.49 | 1367.996 | 1367.996 | 69724.5 | 353.293 | 353.293 | 15486.31 | 12758.17 | 1478.024 |
| H2 | kg/hr | 1844.927 | 7866.336 | 6021.407 | 1844.929 | 7866.336 | 6154.205 | 135.3925 | 6156.802 | 6156.802 | 6018.812 | 2.597229 | 2.597229 | 0.002536 | 0.002536 | 2.594693 | 2.594693 | 6018.812 | 0.002535 | 0.002535 | 1844.927 | 1.39E-06 | 1.65E-31 |
| CO2 | kg/hr | 4232.802 | 31975.15 | 27560.33 | 4414.822 | 31975.15 | 27045.77 | 595.0068 | 28340 | 28340 | 26450.76 | 1294.235 | 1294.235 | 184.6617 | 184.6617 | 1109.574 | 1109.574 | 26450.76 | 182.0199 | 182.0199 | 4232.802 | 2.641795 | 6.60E-24 |
| CO | kg/hr | 8737.46 | 18481.86 | 9744.382 | 8737.476 | 18481.86 | 9955.597 | 219.0231 | 9963.421 | 9963.421 | 9736.574 | 7.82355 | 7.82355 | 0.015618 | 0.015618 | 7.807932 | 7.807932 | 9736.574 | 0.01561 | 0.01561 | 8737.46 | 8.49E-06 | 1.99E-23 |
| CH4 | kg/hr | 506.1319 | 22158.17 | 21651.12 | 507.0475 | 22158.17 | 22053.19 | 485.1702 | 22137.2 | 22137.2 | 21568.02 | 84.01447 | 84.01447 | 0.916257 | 0.916257 | 83.09821 | 83.09821 | 21568.02 | 0.915589 | 0.915589 | 506.1319 | 0.000668 | 0 |
| H2O | kg/hr | 49.51039 | 118.2923 | 68.78013 | 49.51215 | 118.2923 | 58.92972 | 1.296454 | 1546.786 | 1546.786 | 57.63327 | 1487.856 | 1487.856 | 1476.709 | 1476.709 | 11.14686 | 11.14686 | 57.63327 | 0.00176 | 0.00176 | 49.51039 | 0.363954 | 1476.344 |
| N2 | kg/hr | 115.4836 | 5156.235 | 5040.745 | 115.4901 | 5156.235 | 5150.398 | 113.3088 | 5154.06 | 5154.06 | 5037.09 | 3.661842 | 3.661842 | 0.006545 | 0.006545 | 3.655297 | 3.655297 | 5037.09 | 0.006542 | 0.006542 | 115.4836 | 2.50E-06 | 7.49E-20 |
| CH3OH | kg/hr | 0 | 1176.063 | 1005.732 | 170.331 | 1176.063 | 874.8599 | 19.24692 | 13952.16 | 13952.16 | 855.613 | 13077.3 | 13077.3 | 12927.18 | 12927.18 | 150.119 | 150.119 | 855.613 | 170.331 | 170.331 | 0 | 12755.16 | 1.680597 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | | | | | |
| H2 | | 0.119133 | 0.090488 | 0.084698 | 0.116476 | 0.090488 | 0.086323 | 0.086323 | 0.070565 | 0.070565 | 0.086323 | 0.000163 | 0.000163 | 1.74E-07 | 1.74E-07 | 0.001897 | 0.001897 | 0.086323 | 7.17E-06 | 7.17E-06 | 0.119133 | 1.09E-10 | 1.12E-34 |
| CO2 | | 0.273325 | 0.367818 | 0.387669 | 0.27872 | 0.367818 | 0.379361 | 0.379361 | 0.324812 | 0.324812 | 0.379361 | 0.081105 | 0.081105 | 0.012657 | 0.012657 | 0.811094 | 0.811094 | 0.379361 | 0.51521 | 0.51521 | 0.273325 | 0.000207 | 4.47E-27 |
| CO | | 0.564205 | 0.212601 | 0.137066 | 0.551622 | 0.212601 | 0.139644 | 0.139644 | 0.114193 | 0.114193 | 0.139644 | 0.00049 | 0.00049 | 1.07E-06 | 1.07E-06 | 0.005708 | 0.005708 | 0.139644 | 4.42E-05 | 4.42E-05 | 0.564205 | 6.65E-10 | 1.34E-26 |
| CH4 | | 0.032683 | 0.25489 | 0.304549 | 0.032011 | 0.25489 | 0.309332 | 0.309332 | 0.25372 | 0.25372 | 0.309332 | 0.005265 | 0.005265 | 6.28E-05 | 6.28E-05 | 0.060744 | 0.060744 | 0.309332 | 0.002592 | 0.002592 | 0.032683 | 5.24E-08 | 0 |
| H2O | | 0.003197 | 0.001361 | 0.000967 | 0.003126 | 0.001361 | 0.000827 | 0.000827 | 0.017728 | 0.017728 | 0.000827 | 0.093239 | 0.093239 | 0.101217 | 0.101217 | 0.008148 | 0.008148 | 0.000827 | 4.98E-06 | 4.98E-06 | 0.003197 | 2.85E-05 | 0.998863 |
| N2 | | 0.007457 | 0.059313 | 0.070904 | 0.007291 | 0.059313 | 0.072243 | 0.072243 | 0.059072 | 0.059072 | 0.072243 | 0.000229 | 0.000229 | 4.49E-07 | 4.49E-07 | 0.002672 | 0.002672 | 0.072243 | 1.85E-05 | 1.85E-05 | 0.007457 | 1.96E-10 | 5.07E-23 |
| CH3OH | | 0 | 0.013529 | 0.014147 | 0.010753 | 0.013529 | 0.012271 | 0.012271 | 0.159909 | 0.159909 | 0.012271 | 0.819509 | 0.819509 | 0.886061 | 0.886061 | 0.109736 | 0.109736 | 0.012271 | 0.482124 | 0.482124 | 0 | 0.999764 | 0.001137 |
| Volume Flow | cum/hr | 36602.51 | 2308.295 | 1367.035 | 509.5275 | 1873.313 | 1392.557 | 30.63625 | 2691.496 | 1408.109 | 1361.92 | 25.63072 | 480.1083 | 24.14897 | 94.93653 | 478.8227 | 22.77719 | 1337.761 | 5.976883 | 253.1595 | 501.248 | 16.73205 | 1.609242 |

*Table 20. Stream Summary for Configuration I "Methanol Synthesis with a Recycle" for catalyst "A".*

| | Units | CFEED | CPROD | F+R | FEED | FEEDCO2 | FEEDH2 | GAS | H2O | HF+R | HMAIN | LIGHT | MAIN | MEOH | OUTPUT | PROD | PURGE | RECYCLE | TMAIN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | |
| From | | MCOMP | COOL1 | MIX2 | MIX1 | | | CD | CD | HEATFEED | HEATMAIN | FLASH1 | MIXMAIN | CD | FLASH1 | R1 | MIX3 | MIX3 | PUMP |
| To | | MIX2 | FLASH1 | HEATFEED | MCOMP | MIX1 | MIX1 | MIX1 | | R1 | PUMP | MIX3 | HEATMAIN | | MIXMAIN | COOL1 | | MIX2 | CD |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | | | - 471.151 | 4 616.122 | | - | | | | | 6 295.833 | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | |
| Phase | | Vapor Phase | | Vapor Phase | Vapor Phase | Vapor Phase | Vapor Phase | Vapor Phase | Liquid Phase | Vapor Phase | Liquid Phase | Vapor Phase | Liquid Phase | Liquid Phase | Liquid Phase | Vapor Phase | Vapor Phase | Vapor Phase | Liquid Phase |
| Temperature | C | 177.53 | 5.00 | 58.60 | 25.65 | 25.00 | 25.00 | 15.16 | 93.52 | 255.00 | 38.00 | 5.00 | 5.00 | 15.16 | 5.00 | 255.00 | 5.00 | 5.00 | 33.49 |
| Pressure | bar | 100.00 | 100.00 | 100.00 | 0.80 | 1.00 | 35.00 | 0.80 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 5.38 |
| Molar Vapor Fraction | | 1.000 | 0.836 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | - | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Molar Liquid Fraction | | - | 0.164 | - | - | - | - | - | 1.000 | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Mass Vapor Fraction | | 1.000 | 0.564 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | - | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Mass Liquid Fraction | | - | 0.436 | 0.000 | - | - | - | - | 1.000 | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Molar Enthalpy | kcal/mol | - 22.15 | - 18.53 | - 13.28 | - 23.31 | - 94.00 | 0.01 | - 86.46 | - 67.00 | - 11.79 | - 62.95 | - 9.59 | - 64.21 | - 57.17 | - 64.21 | - 14.87 | - 9.59 | - 9.59 | - 62.99 |
| Mass Enthalpy | kcal/kg | - 1 780.30 | - 1 953.23 | - 1 625.24 | - 1 873.72 | - 2 135.84 | 4.73 | - 2 074.92 | - 3 718.84 | - 1 442.04 | - 2 489.35 | - 1 499.55 | - 2 539.06 | - 1 783.85 | - 2 539.06 | - 1 566.78 | - 1 499.55 | - 1 499.55 | - 2 490.81 |
| Molar Entropy | cal/mol-K | - 4.78 | - 15.54 | - 7.30 | 1.75 | 0.69 | - 7.04 | - 2.10 | - 35.18 | - 3.76 | - 46.27 | - 8.69 | - 50.51 | - 58.03 | - 50.51 | - 6.15 | - 8.69 | - 8.69 | - 46.29 |
| Mass Entropy | cal/gm-K | - 0.38 | - 1.64 | - 0.89 | 0.14 | 0.02 | - 3.49 | - 0.05 | - 1.95 | - 0.46 | - 1.83 | - 1.36 | - 2.00 | - 1.81 | - 2.00 | - 0.65 | - 1.36 | - 1.36 | - 1.83 |
| Molar Density | mol/cc | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.03 | 0.00 | 0.03 | 0.03 | 0.03 | 0.00 | 0.00 | 0.00 | 0.03 |
| Mass Density | kg/cum | 31.84 | 45.49 | 28.23 | 0.40 | 1.78 | 2.79 | 1.39 | 925.11 | 17.90 | 838.10 | 26.23 | 875.07 | 804.65 | 875.07 | 20.91 | 26.23 | 26.23 | 843.27 |
| Enthalpy Flow | Gcal/hr | - 36.91 | - 90.44 | - 75.25 | - 38.84 | - 37.77 | 0.01 | - 1.09 | - 26.37 | - 66.77 | - 50.30 | - 39.13 | - 51.31 | - 22.46 | - 51.31 | - 72.55 | - 0.78 | - 38.35 | - 50.33 |
| Average MW | | 12.44 | 9.49 | 8.17 | 12.44 | 44.01 | 2.02 | 41.67 | 18.02 | 8.17 | 25.29 | 6.40 | 25.29 | 32.05 | 25.29 | 9.49 | 6.40 | 6.40 | 25.29 |
| Mole Flows | kmol/hr | 1 666.16 | 4 879.52 | 5 664.95 | 1 666.16 | 401.77 | 1 251.80 | 12.59 | 393.64 | 5 664.95 | 799.12 | 4 080.40 | 799.12 | 392.89 | 799.12 | 4 879.52 | 81.61 | 3 998.79 | 799.12 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.2476 | 0.0834 | 0.1413 | 0.2476 | 1.0000 | - | 0.8560 | 0.0000 | 0.1413 | 0.0138 | 0.0971 | 0.0138 | 0.0005 | 0.0138 | 0.0834 | 0.0971 | 0.0971 | 0.0138 |
| H2 | | 0.7515 | 0.7454 | 0.8502 | 0.7515 | - | 1.0000 | 0.0205 | 0.0000 | 0.8502 | 0.0003 | 0.8913 | 0.0003 | 0.0000 | 0.0003 | 0.7454 | 0.8913 | 0.8913 | 0.0003 |
| CH3OH | | 0.0009 | 0.0811 | 0.0005 | 0.0009 | - | - | 0.1230 | 0.0000 | 0.0005 | 0.4933 | 0.0004 | 0.4933 | 0.9995 | 0.4933 | 0.0811 | 0.0004 | 0.0004 | 0.4933 |
| H2O | | 0.0000 | 0.0807 | 0.0000 | 0.0000 | - | - | 0.0000 | 1.0000 | 0.0000 | 0.4926 | 0.0001 | 0.4926 | 0.0000 | 0.4926 | 0.0807 | 0.0001 | 0.0001 | 0.4926 |
| CO | | 0.0000 | 0.0093 | 0.0079 | 0.0000 | - | - | 0.0005 | 0.0000 | 0.0079 | 0.0000 | 0.0112 | 0.0000 | 0.0000 | 0.0000 | 0.0093 | 0.0112 | 0.0112 | 0.0000 |
| Mass Flows | kg/hr | 20 729.78 | 46 302.27 | 46 302.27 | 20 729.78 | 17 681.64 | 2 523.48 | 524.65 | 7 091.66 | 46 302.27 | 20 207.98 | 26 094.29 | 20 207.98 | 12 591.67 | 20 207.98 | 46 302.27 | 521.89 | 25 572.40 | 20 207.98 |
| CO2 | kg/hr | 18 155.99 | 17 916.57 | 35 240.14 | 18 155.99 | 17 681.64 | - | 474.34 | 0.00 | 35 240.14 | 483.84 | 17 432.74 | 483.84 | 9.49 | 483.84 | 17 916.57 | 348.65 | 17 084.08 | 483.84 |
| H2 | kg/hr | 2 524.00 | 7 332.17 | 9 709.03 | 2 524.00 | - | 2 523.48 | 0.52 | 0.00 | 9 709.03 | 0.52 | 7 331.65 | 0.52 | 0.00 | 0.52 | 7 332.17 | 146.63 | 7 185.02 | 0.52 |
| CH3OH | kg/hr | 49.62 | 12 681.40 | 97.86 | 49.62 | - | - | 49.62 | 0.39 | 97.86 | 12 632.18 | 49.23 | 12 632.18 | 12 582.17 | 12 632.18 | 12 681.40 | 0.98 | 48.24 | 12 632.18 |
| H2O | kg/hr | 0.00 | 7 095.31 | 3.96 | 0.00 | - | - | 0.00 | 7 091.27 | 3.96 | 7 091.27 | 4.04 | 7 091.27 | 0.01 | 7 091.27 | 7 095.31 | 0.08 | 3.96 | 7 091.27 |
| CO | kg/hr | 0.17 | 1 276.80 | 1 251.27 | 0.17 | - | - | 0.17 | 0.00 | 1 251.27 | 0.17 | 1 276.63 | 0.17 | 0.00 | 0.17 | 1 276.80 | 25.53 | 1 251.10 | 0.17 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.8758 | 0.3869 | 0.7611 | 0.8758 | 1.0000 | - | 0.9041 | 0.0000 | 0.7611 | 0.0239 | 0.6681 | 0.0239 | 0.0008 | 0.0239 | 0.3869 | 0.6681 | 0.6681 | 0.0239 |
| H2 | | 0.1218 | 0.1584 | 0.2097 | 0.1218 | - | 1.0000 | 0.0010 | 0.0000 | 0.2097 | 0.0000 | 0.2810 | 0.0000 | 0.0000 | 0.0000 | 0.1584 | 0.2810 | 0.2810 | 0.0000 |
| CH3OH | | 0.0024 | 0.2739 | 0.0021 | 0.0024 | - | - | 0.0946 | 0.0001 | 0.0021 | 0.6251 | 0.0019 | 0.6251 | 0.9992 | 0.6251 | 0.2739 | 0.0019 | 0.0019 | 0.6251 |
| H2O | | 0.0000 | 0.1532 | 0.0001 | 0.0000 | - | - | 0.0000 | 0.9999 | 0.0001 | 0.3509 | 0.0002 | 0.3509 | 0.0000 | 0.3509 | 0.1532 | 0.0002 | 0.0002 | 0.3509 |
| CO | | 0.0000 | 0.0276 | 0.0270 | 0.0000 | - | - | 0.0003 | 0.0000 | 0.0270 | 0.0000 | 0.0489 | 0.0000 | 0.0000 | 0.0000 | 0.0276 | 0.0489 | 0.0489 | 0.0000 |
| Volume Flow | cum/hr | 651.0 | 1 017.8 | 1 640.0 | 51 749.7 | 9 910.2 | 905.2 | 377.3 | 7.7 | 2 586.6 | 24.1 | 994.7 | 23.1 | 15.6 | 23.1 | 2 213.9 | 19.9 | 974.8 | 24.0 |

*Table 21. Stream Summary for Configuration II "Methanol Synthesis with Two Reactors in Series" for catalyst "A".*

| | Units | CMAIN | F+R | FEEDCO2 | FEEDH2 | GAS | H2O | HLIGHT | HPROD | HPROD2 | LIGHT | LIGHT2 | MAIN | MCS4H | MEOH | OUTPUT | OUTPUT2 | PROD | PROD2 | PURGE | S2 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | | | |
| From | | B5 | MIX1 | | | CD | CD | COOL2 | COOL1 | COOL3 | FLASH1 | FLASH2 | MIXMAIN | MCOMP | CD | FLASH1 | FLASH2 | R1 | R2 | B6 | HMAIN |
| To | | CD | MCOMP | MIX1 | MIX1 | B6 | | R2 | FLASH1 | FLASH2 | COOL2 | B6 | HMAIN | R1 | | MIXMAIN | MIXMAIN | COOL1 | COOL3 | | B5 |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | - 596.5 | 11 283.1 | | - | | | | | | | | 6 211.5 | | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | | | |
| Phase | | Liquid Phase | Vapor Phase | Vapor Phase | Vapor Phase | Vapor Phas | Liquid Phas | Vapor Phase | | | Vapor Phase | Vapor Phase | | Vapor Phase | Liquid Phase | Liquid Phase | Liquid Phas | Vapor Phase | Vapor Phase | Vapor Phase | Liquid Phase |
| Temperature | C | 27.48 | 25.98 | 25.00 | 25.00 | 13.07 | 93.52 | 255.00 | 5.00 | 5.00 | 5.00 | 5.00 | 5.00 | 255.00 | 13.07 | 5.00 | 5.00 | 255.00 | 255.00 | 6.46 | 31.00 |
| Pressure | bar | 1.00 | 1.00 | 1.00 | 35.00 | 0.80 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 |
| Molar Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 0.838 | 0.869 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Molar Liquid Fraction | | 1.000 | - | - | - | - | 1.000 | - | 0.162 | 0.131 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Mass Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 0.564 | 0.526 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Mass Liquid Fraction | | 1.000 | - | - | - | - | 1.000 | - | 0.436 | 0.474 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Molar Enthalpy | kcal/mol | - 63.12 | - 13.39 | - 94.00 | 0.01 | - 86.44 | - 67.00 | - 7.33 | - 18.11 | - 12.62 | - 9.18 | - 4.90 | - 64.20 | - 11.66 | - 57.22 | - 64.44 | - 63.81 | - 14.47 | - 9.34 | - 5.26 | - 63.08 |
| Mass Enthalpy | kcal/kg | - 2 518.03 | - 1 673.45 | - 2 135.84 | 4.73 | - 2 081.23 | - 3 718.95 | - 1 181.64 | - 1 965.52 | - 1 793.60 | - 1 480.48 | - 1 149.69 | - 2 561.10 | - 1 457.47 | - 1 785.68 | - 2 592.95 | - 2 509.13 | - 1 569.83 | - 1 327.58 | - 1 188.75 | - 2 516.52 |
| Molar Entropy | cal/mol-K | - 46.72 | 0.96 | 0.69 | - 7.04 | - 1.73 | - 35.18 | - 3.98 | - 15.42 | - 14.53 | - 8.73 | - 9.01 | - 50.47 | - 4.00 | - 58.15 | - 50.07 | - 51.14 | - 6.09 | - 6.08 | 0.71 | - 46.67 |
| Mass Entropy | cal/gm-K | - 1.86 | 0.12 | 0.02 | - 3.49 | - 0.04 | - 1.95 | - 0.64 | - 1.67 | - 2.07 | - 1.41 | - 2.12 | - 2.01 | - 0.50 | - 1.81 | - 2.01 | - 2.01 | - 0.66 | - 0.86 | 0.16 | - 1.86 |
| Molar Density | mol/cc | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.00 | 0.03 | 0.04 | 0.03 | 0.00 | 0.00 | 0.00 | 0.03 |
| Mass Density | kg/cum | 850.65 | 0.32 | 1.78 | 2.79 | 1.40 | 925.12 | 13.59 | 44.08 | 32.43 | 25.42 | 17.38 | 875.44 | 17.53 | 807.13 | 879.03 | 869.74 | 20.31 | 15.45 | 0.15 | 846.69 |
| Enthalpy Flow | Gcal/hr | - 51.17 | - 48.37 | - 48.40 | 0.03 | - 0.78 | - 27.42 | - 19.26 | - 56.81 | - 29.24 | - 24.13 | - 9.86 | - 52.05 | - 42.12 | - 22.45 | - 32.68 | - 19.37 | - 45.37 | - 21.64 | - 10.65 | - 51.14 |
| Average MW | | 25.07 | 8.00 | 44.01 | 2.02 | 41.53 | 18.02 | 6.20 | 9.21 | 7.03 | 6.20 | 4.26 | 25.07 | 8.00 | 32.04 | 24.85 | 25.43 | 9.21 | 7.03 | 4.43 | 25.07 |
| Mole Flows | kmol/hr | 810.70 | 3 611.93 | 514.87 | 3 097.06 | 9.04 | 409.24 | 2 629.51 | 3 136.61 | 2 317.39 | 2 629.51 | 2 013.79 | 810.70 | 3 611.93 | 392.42 | 507.10 | 303.60 | 3 136.61 | 2 317.39 | 2 022.83 | 810.70 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0099 | 0.1425 | 1.0000 | - | 0.8627 | 0.0000 | 0.0930 | 0.0798 | 0.0430 | 0.0930 | 0.0483 | 0.0099 | 0.1425 | 0.0006 | 0.0112 | 0.0077 | 0.0798 | 0.0430 | 0.0520 | 0.0099 |
| H2 | | 0.0003 | 0.8575 | - | 1.0000 | 0.0277 | 0.0000 | 0.8963 | 0.7515 | 0.8199 | 0.8963 | 0.9434 | 0.0003 | 0.8575 | 0.0000 | 0.0003 | 0.0004 | 0.7515 | 0.8199 | 0.9393 | 0.0003 |
| CH3OH | | 0.4848 | - | - | - | 0.1091 | 0.0000 | 0.0004 | 0.0758 | 0.0678 | 0.0004 | 0.0003 | 0.4848 | - | 0.9990 | 0.4668 | 0.5148 | 0.0758 | 0.0678 | 0.0008 | 0.4848 |
| H2O | | 0.5050 | - | - | - | 0.0000 | 1.0000 | 0.0001 | 0.0844 | 0.0625 | 0.0001 | 0.0000 | 0.5050 | - | 0.0004 | 0.5217 | 0.4771 | 0.0844 | 0.0625 | 0.0000 | 0.5050 |
| CO | | 0.0000 | - | - | - | 0.0005 | 0.0000 | 0.0103 | 0.0086 | 0.0068 | 0.0103 | 0.0078 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0086 | 0.0068 | 0.0078 | 0.0000 |
| Mass Flows | kg/hr | 20 322.64 | 28 902.49 | 22 659.19 | 6 243.30 | 375.55 | 7 372.57 | 16 300.88 | 28 902.49 | 16 300.88 | 16 300.88 | 8 579.85 | 20 322.64 | 28 902.49 | 12 574.52 | 12 601.61 | 7 721.03 | 28 902.49 | 16 300.88 | 8 955.41 | 20 322.64 |
| CO2 | kg/hr | 353.51 | 22 659.19 | 22 659.19 | - | 343.31 | 0.00 | 10 758.84 | 11 009.31 | 4 386.61 | 10 758.84 | 4 283.57 | 353.51 | 22 659.19 | 10.21 | 250.47 | 103.04 | 11 009.31 | 4 386.61 | 4 626.88 | 353.51 |
| H2 | kg/hr | 0.50 | 6 243.30 | - | 6 243.30 | 0.50 | 0.00 | 4 751.22 | 4 751.50 | 3 830.14 | 4 751.22 | 3 829.92 | 0.50 | 6 243.30 | 0.00 | 0.28 | 0.22 | 4 751.50 | 3 830.14 | 3 830.42 | 0.50 |
| CH3OH | kg/hr | 12 592.97 | - | - | - | 31.61 | 0.00 | 30.46 | 7 615.05 | 5 030.95 | 30.46 | 22.58 | 12 592.97 | - | 12 561.36 | 7 584.60 | 5 008.37 | 7 615.05 | 5 030.95 | 54.19 | 12 592.97 |
| H2O | kg/hr | 7 375.52 | - | - | - | 0.00 | 7 372.57 | 2.66 | 4 768.85 | 2 611.11 | 2.66 | 1.77 | 7 375.52 | - | 2.95 | 4 766.18 | 2 609.34 | 4 768.85 | 2 611.11 | 1.77 | 7 375.52 |
| CO | kg/hr | 0.13 | - | - | - | 0.13 | 0.00 | 757.71 | 757.79 | 442.06 | 757.71 | 442.01 | 0.13 | - | 0.00 | 0.08 | 0.05 | 757.79 | 442.06 | 442.14 | 0.13 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0174 | 0.7840 | 1.0000 | - | 0.9141 | 0.0000 | 0.6600 | 0.3809 | 0.2691 | 0.6600 | 0.4993 | 0.0174 | 0.7840 | 0.0008 | 0.0199 | 0.0133 | 0.3809 | 0.2691 | 0.5167 | 0.0174 |
| H2 | | 0.0000 | 0.2160 | - | 1.0000 | 0.0013 | 0.0000 | 0.2915 | 0.1644 | 0.2350 | 0.2915 | 0.4464 | 0.0000 | 0.2160 | 0.0000 | 0.0000 | 0.0000 | 0.1644 | 0.2350 | 0.4277 | 0.0000 |
| CH3OH | | 0.6197 | - | - | - | 0.0842 | 0.0000 | 0.0019 | 0.2635 | 0.3086 | 0.0019 | 0.0026 | 0.6197 | - | 0.9990 | 0.6019 | 0.6487 | 0.2635 | 0.3086 | 0.0061 | 0.6197 |
| H2O | | 0.3629 | - | - | - | 0.0000 | 1.0000 | 0.0002 | 0.1650 | 0.1602 | 0.0002 | 0.0002 | 0.3629 | - | 0.0002 | 0.3782 | 0.3380 | 0.1650 | 0.1602 | 0.0002 | 0.3629 |
| CO | | 0.0000 | - | - | - | 0.0003 | 0.0000 | 0.0465 | 0.0262 | 0.0271 | 0.0465 | 0.0515 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0262 | 0.0271 | 0.0494 | 0.0000 |
| Volume Flow | cum/hr | 23.9 | 89 872.0 | 12 700.0 | 2 239.5 | 269.0 | 8.0 | 1 199.2 | 655.7 | 502.6 | 641.4 | 493.7 | 23.2 | 1 648.9 | 15.6 | 14.3 | 8.9 | 1 423.3 | 1 054.8 | 58 810.5 | 24.0 |

*Table 22. Stream Summary for Configuration III "Methanol Synthesis with Two Reactors in Series with a Recycle" for catalyst "A".*

| | Units | CMAIN | F+R | FEED | FEEDCO2 | FEEDH2 | GAS | H2O | HF+R | HLIGHT | HMAIN | HPROD | HPROD2 | LIGHT | LIGHT2 | MAIN | MCS4H | MEOH | OUTPUT | OUTPUT2 | PROD | PROD2 | PURGE | RECYCLE |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | | | | | | |
| From | | TURB3 | MIX2 | MIX1 | | | CD | CD | HEAT1 | HEAT2 | HEATMAIN | COOL1 | COOL3 | FLASH1 | FLASH2 | MIXMAIN | MCOMP | CD | FLASH1 | FLASH2 | R1 | R2 | MIX3 | MIX3 |
| To | | CD | HEAT1 | MCOMP | MIX1 | MIX1 | MIX1 | | R1 | R2 | TURB3 | FLASH1 | FLASH2 | HEAT2 | MIX3 | HEATMAIN | MIX2 | | MIXMAIN | MIXMAIN | COOL1 | COOL3 | | MIX2 |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | | - 455.22 | 4 401.17 | | | - | | | | | | | | | 6 183.87 | | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | | | | | | |
| Phase | | Liquid Phas | Vapor Phas | Vapor Phas | Vapor Phas | Vapor Pha | Vapor Phas | Liquid Phas | Vapor Phas | Vapor Phas | Liquid Phase | | | Vapor Phas | Vapor Phase | | Vapor Phas | Liquid Phas | Liquid Phas | Liquid Phas | Liquid Phas | Vapor Phas | Vapor Phas | Vapor Phas | Vapor Phas |
| Temperature | C | 25.0 | 126.6 | 25.7 | 25.0 | 25.0 | 15.8 | 93.5 | 255.0 | 255.0 | 25.0 | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 | 255.0 | 15.8 | 5.0 | 5.0 | 255.0 | 255.0 | 5.0 | 5.0 |
| Pressure | bar | 1.0 | 100.0 | 0.8 | 1.0 | 35.0 | 0.8 | 0.8 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 0.8 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 |
| Molar Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 1.000 | - | 0.837 | 0.867 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | 1.000 |
| Molar Liquid Fraction | | 1.000 | - | - | - | - | - | 1.000 | - | - | 1.000 | 0.163 | 0.133 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | - |
| Mass Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 1.000 | - | 0.564 | 0.527 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | 1.000 |
| Mass Liquid Fraction | | 1.000 | 0.000 | - | - | - | - | 1.000 | - | - | 1.000 | 0.436 | 0.473 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | - |
| Molar Enthalpy | kcal/mol | - 63.1 | - 12.7 | - 23.5 | - 94.0 | 0.0 | - 85.7 | - 67.0 | - 11.7 | - 7.6 | - 63.1 | - 18.3 | - 13.0 | - 9.4 | - 5.1 | - 64.1 | - 21.7 | - 57.2 | - 64.3 | - 63.8 | - 14.7 | - 9.6 | - 5.1 | - 5.1 |
| Mass Enthalpy | kcal/kg | - 2 501.1 | - 1 569.8 | - 1 875.7 | - 2 135.8 | 4.7 | - 2 071.5 | - 3 718.8 | - 1 448.8 | - 1 197.6 | - 2 499.6 | - 1 958.1 | - 1 804.4 | - 1 491.5 | - 1 174.3 | - 2 540.5 | - 1 732.4 | - 1 783.4 | - 2 561.2 | - 2 506.6 | - 1 567.8 | - 1 343.9 | - 1 174.3 | - 1 174.3 |
| Molar Entropy | cal/mol-K | - 47.2 | - 6.0 | 1.8 | 0.7 | - 7.0 | - 2.2 | - 35.2 | - 3.9 | - 4.0 | - 47.0 | - 15.5 | - 14.6 | - 8.7 | - 9.0 | - 50.6 | - 3.5 | - 58.0 | - 50.3 | - 51.1 | - 6.1 | - 6.1 | - 9.0 | - 9.0 |
| Mass Entropy | cal/gm-K | - 1.9 | - 0.7 | 0.1 | 0.0 | - 3.5 | - 0.1 | - 2.0 | - 0.5 | - 0.6 | - 1.9 | - 1.7 | - 2.0 | - 1.4 | - 2.1 | - 2.0 | - 0.3 | - 1.8 | - 2.0 | - 2.0 | - 0.7 | - 0.8 | - 2.1 | - 2.1 |
| Molar Density | mol/cc | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Mass Density | kg/cum | 851.9 | 23.3 | 0.4 | 1.8 | 2.8 | 1.4 | 925.1 | 17.7 | 13.8 | 851.9 | 44.9 | 33.2 | 25.9 | 17.8 | 874.0 | 27.4 | 803.9 | 876.7 | 869.7 | 20.7 | 15.8 | 17.8 | 17.8 |
| Enthalpy Flow | Gcal/hr | - 50.0 | - 44.6 | - 37.8 | - 36.9 | 0.0 | - 0.9 | - 26.2 | - 41.2 | - 19.2 | - 49.9 | - 55.6 | - 28.9 | - 23.9 | - 9.9 | - 50.7 | - 34.9 | - 22.3 | - 31.7 | - 19.0 | - 44.6 | - 21.5 | - 0.2 | - 9.7 |
| Average MW | | 25.2 | 8.1 | 12.5 | 44.0 | 2.0 | 41.4 | 18.0 | 8.1 | 6.3 | 25.2 | 9.4 | 7.2 | 6.3 | 4.4 | 25.2 | 12.5 | 32.0 | 25.1 | 25.5 | 9.4 | 7.2 | 4.4 | 4.4 |
| Mole Flows | kmol/hr | 791.38 | 3 507.07 | 1 610.98 | 392.92 | 1 208.06 | 10.00 | 390.77 | 3 507.07 | 2 539.10 | 791.38 | 3 032.80 | 2 232.49 | 2 539.10 | 1 934.81 | 791.38 | 1 610.98 | 390.61 | 493.70 | 297.68 | 3 032.80 | 2 232.49 | 38.70 | 1 896.12 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0110 | 0.1419 | 0.2492 | 1.0000 | - | 0.8459 | 0.0000 | 0.1419 | 0.0953 | 0.0110 | 0.0819 | 0.0450 | 0.0953 | 0.0507 | 0.0110 | 0.2492 | 0.0005 | 0.0126 | 0.0081 | 0.0819 | 0.0450 | 0.0507 | 0.0507 |
| H2 | | 0.0003 | 0.8532 | 0.7501 | - | 1.0000 | 0.0259 | 0.0000 | 0.8532 | 0.8935 | 0.0003 | 0.7481 | 0.8154 | 0.8935 | 0.9408 | 0.0003 | 0.7501 | 0.0000 | 0.0003 | 0.0004 | 0.7481 | 0.8154 | 0.9408 | 0.9408 |
| CH3OH | | 0.4950 | 0.0006 | 0.0008 | - | - | 0.1277 | 0.0000 | 0.0006 | 0.0004 | 0.4950 | 0.0788 | 0.0691 | 0.0004 | 0.0004 | 0.4950 | 0.0008 | 0.9995 | 0.4823 | 0.5159 | 0.0788 | 0.0691 | 0.0004 | 0.0004 |
| H2O | | 0.4938 | 0.0000 | 0.0000 | - | - | 0.0000 | 1.0000 | 0.0000 | 0.0001 | 0.4938 | 0.0822 | 0.0635 | 0.0001 | 0.0000 | 0.4938 | 0.0000 | 0.0000 | 0.5047 | 0.4756 | 0.0822 | 0.0635 | 0.0000 | 0.0000 |
| CO | | 0.0000 | 0.0044 | 0.0000 | - | - | 0.0005 | 0.0000 | 0.0044 | 0.0108 | 0.0000 | 0.0090 | 0.0070 | 0.0108 | 0.0081 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0090 | 0.0070 | 0.0081 | 0.0081 |
| Mass Flows | kg/hr | 19 972.43 | 28 418.79 | 20 141.38 | 17 292.23 | 2 435.31 | 413.84 | 7 040.04 | 28 418.79 | 16 024.32 | 19 972.43 | 28 418.79 | 16 024.32 | 16 024.32 | 8 446.36 | 19 972.43 | 20 141.38 | 12 518.56 | 12 394.47 | 7 577.97 | 28 418.79 | 16 024.32 | 168.93 | 8 277.43 |
| CO2 | kg/hr | 381.40 | 21 893.94 | 17 664.50 | 17 292.23 | - | 372.26 | 0.00 | 21 893.94 | 10 651.18 | 381.40 | 10 926.00 | 4 422.29 | 10 651.18 | 4 315.71 | 381.40 | 17 664.50 | 9.14 | 274.82 | 106.58 | 10 926.00 | 4 422.29 | 86.31 | 4 229.40 |
| H2 | kg/hr | 0.52 | 6 032.00 | 2 435.83 | - | 2 435.31 | 0.52 | 0.00 | 6 032.00 | 4 573.24 | 0.52 | 4 573.54 | 3 669.84 | 4 573.24 | 3 669.62 | 0.52 | 2 435.83 | 0.00 | 0.30 | 0.22 | 4 573.54 | 3 669.84 | 73.39 | 3 596.23 |
| CH3OH | kg/hr | 12 550.93 | 62.29 | 40.91 | - | - | 40.91 | 0.62 | 62.29 | 30.12 | 12 550.93 | 7 660.54 | 4 942.33 | 30.12 | 21.83 | 12 550.93 | 40.91 | 12 509.40 | 7 630.43 | 4 920.50 | 7 660.54 | 4 942.33 | 0.44 | 21.39 |
| H2O | kg/hr | 7 039.44 | 1.67 | 0.00 | - | - | 0.00 | 7 039.42 | 1.67 | 2.54 | 7 039.44 | 4 491.37 | 2 552.32 | 2.54 | 1.71 | 7 039.44 | 0.00 | 0.02 | 4 488.83 | 2 550.61 | 4 491.37 | 2 552.32 | 0.03 | 1.67 |
| CO | kg/hr | 0.15 | 428.89 | 0.15 | - | - | 0.15 | 0.00 | 428.89 | 767.25 | 0.15 | 767.34 | 437.55 | 767.25 | 437.49 | 0.15 | 0.15 | 0.00 | 0.09 | 0.05 | 767.34 | 437.55 | 8.75 | 428.74 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0191 | 0.7704 | 0.8770 | 1.0000 | - | 0.8995 | 0.0000 | 0.7704 | 0.6647 | 0.0191 | 0.3845 | 0.2760 | 0.6647 | 0.5110 | 0.0191 | 0.8770 | 0.0007 | 0.0222 | 0.0141 | 0.3845 | 0.2760 | 0.5110 | 0.5110 |
| H2 | | 0.0000 | 0.2123 | 0.1209 | - | 1.0000 | 0.0013 | 0.0000 | 0.2123 | 0.2854 | 0.0000 | 0.1609 | 0.2290 | 0.2854 | 0.4345 | 0.0000 | 0.1209 | 0.0000 | 0.0000 | 0.0000 | 0.1609 | 0.2290 | 0.4345 | 0.4345 |
| CH3OH | | 0.6284 | 0.0022 | 0.0020 | - | - | 0.0988 | 0.0001 | 0.0022 | 0.0019 | 0.6284 | 0.2696 | 0.3084 | 0.0019 | 0.0026 | 0.6284 | 0.0020 | 0.9993 | 0.6156 | 0.6493 | 0.2696 | 0.3084 | 0.0026 | 0.0026 |
| H2O | | 0.3525 | 0.0001 | 0.0000 | - | - | 0.0000 | 0.9999 | 0.0001 | 0.0002 | 0.3525 | 0.1580 | 0.1593 | 0.0002 | 0.0002 | 0.3525 | 0.0000 | 0.0000 | 0.3622 | 0.3366 | 0.1580 | 0.1593 | 0.0002 | 0.0002 |
| CO | | 0.0000 | 0.0151 | 0.0000 | - | - | 0.0004 | 0.0000 | 0.0151 | 0.0479 | 0.0000 | 0.0270 | 0.0273 | 0.0479 | 0.0518 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0270 | 0.0273 | 0.0518 | 0.0518 |
| Volume Flow | cum/hr | 23.45 | 1 220.89 | 50 038.56 | 9 691.91 | 873.57 | 300.30 | 7.61 | 1 601.20 | 1 158.11 | 23.44 | 633.25 | 482.95 | 619.11 | 474.24 | 22.85 | 736.11 | 15.57 | 14.14 | 8.71 | 1 376.11 | 1 016.02 | 9.48 | 464.75 |

*Table 23. Stream Summary for Configuration I "Methanol Synthesis with a Recycle" for catalyst "B".*

| | Units | CFEED | CPROD | F+R | FEED | FEEDCO2 | FEEDH2 | GAS | H2O | HF+R | HMAIN | LIGHT | MAIN | MEOH | OUTPUT | PROD | PURGE | RECYCLE | TMAIN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | |
| From | | MCOMP | COOL1 | MIX2 | MIX1 | | | CD | CD | HEATFEED | HEATMAIN | FLASH1 | MIXMAIN | CD | FLASH1 | R1 | MIX3 | MIX3 | PUMP |
| To | | MIX2 | FLASH1 | HEATFEED | MCOMP | MIX1 | MIX1 | MIX1 | | R1 | PUMP | MIX3 | HEATMAIN | | MIXMAIN | COOL1 | | MIX2 | CD |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | | | - 453.39 | 4 361.31 | | - | | | | | 6 186.61 | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | |
| Phase | | Vapor Phase | | Vapor Phase | Vapor Phase | Vapor Phase | Vapor Phas | Vapor Phas | Liquid Phas | Vapor Phase | Liquid Phase | Vapor Phas | Liquid Phase | Liquid Phase | Liquid Phase | Vapor Phase | Vapor Pha | Vapor Phas | Liquid Phase |
| Temperature | C | 177.62 | 5.00 | 107.85 | 25.78 | 25.00 | 25.00 | 48.18 | 93.52 | 232.00 | 32.00 | 5.00 | 5.00 | 48.18 | 5.00 | 232.00 | 5.00 | 5.00 | 30.12 |
| Pressure | bar | 100.00 | 100.00 | 100.00 | 0.80 | 1.00 | 35.00 | 0.80 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 5.00 |
| Molar Vapor Fraction | | 1.000 | 0.612 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | - | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Molar Liquid Fraction | | - | 0.388 | - | - | - | - | - | 1.000 | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Mass Vapor Fraction | | 1.000 | 0.141 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | - | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Mass Liquid Fraction | | - | 0.859 | - | - | - | - | - | 1.000 | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Molar Enthalpy | kcal/mol | - 22.03 | - 25.29 | - 12.89 | - 23.19 | - 94.00 | 0.01 | - 52.09 | - 67.00 | - 11.95 | - 62.61 | - 0.93 | - 63.79 | - 56.41 | - 63.79 | - 19.47 | - 0.93 | - 0.93 | - 62.65 |
| Mass Enthalpy | kcal/kg | - 1 778.35 | - 2 239.25 | - 1 582.47 | - 1 872.16 | - 2 135.84 | 4.73 | - 1 683.34 | - 3 718.95 | - 1 466.24 | - 2 500.25 | - 358.51 | - 2 547.37 | - 1 760.49 | - 2 547.37 | - 1 724.19 | - 358.51 | - 358.51 | - 2 501.70 |
| Molar Entropy | cal/mol-K | - 4.78 | - 25.38 | - 6.29 | 1.75 | 0.69 | - 7.04 | - 16.59 | - 35.18 | - 4.14 | - 47.07 | - 9.11 | - 51.10 | - 55.74 | - 51.10 | - 10.98 | - 9.11 | - 9.11 | - 47.18 |
| Mass Entropy | cal/gm-K | - 0.39 | - 2.25 | - 0.77 | 0.14 | 0.02 | - 3.49 | - 0.54 | - 1.95 | - 0.51 | - 1.88 | - 3.51 | - 2.04 | - 1.74 | - 2.04 | - 0.97 | - 3.51 | - 3.51 | - 1.88 |
| Molar Density | mol/cc | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.03 | 0.00 | 0.03 | 0.02 | 0.03 | 0.00 | 0.00 | 0.00 | 0.03 |
| Mass Density | kg/cum | 31.69 | 69.81 | 24.53 | 0.40 | 1.78 | 2.79 | 0.93 | 925.12 | 18.63 | 840.57 | 10.55 | 870.16 | 764.75 | 870.16 | 27.45 | 10.55 | 10.55 | 842.67 |
| Enthalpy Flow | Gcal/hr | - 34.61 | - 50.55 | - 35.73 | - 36.43 | - 36.34 | 0.01 | - 0.10 | - 25.89 | - 33.10 | - 48.50 | - 1.14 | - 49.41 | - 21.78 | - 49.41 | - 38.93 | - 0.02 | - 1.12 | - 48.53 |
| Average MW | | 12.39 | 11.29 | 8.15 | 12.39 | 44.01 | 2.02 | 30.94 | 18.02 | 8.15 | 25.04 | 2.60 | 25.04 | 32.04 | 25.04 | 11.29 | 2.60 | 2.60 | 25.04 |
| Mole Flows | kmol/hr | 1 571.33 | 1 998.79 | 2 771.04 | 1 571.33 | 386.62 | 1 182.70 | 2.01 | 386.48 | 2 771.04 | 774.64 | 1 224.16 | 774.64 | 386.15 | 774.64 | 1 998.79 | 24.48 | 1 199.67 | 774.64 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.2463 | 0.0029 | 0.1415 | 0.2463 | 1.0000 | - | 0.2284 | 0.0000 | 0.1415 | 0.0006 | 0.0043 | 0.0006 | 0.0001 | 0.0006 | 0.0029 | 0.0043 | 0.0043 | 0.0006 |
| H2 | | 0.7528 | 0.6005 | 0.8513 | 0.7528 | - | 1.0000 | 0.1271 | 0.0000 | 0.8513 | 0.0003 | 0.9803 | 0.0003 | 0.0000 | 0.0003 | 0.6005 | 0.9803 | 0.9803 | 0.0003 |
| CH3OH | | 0.0008 | 0.1940 | 0.0006 | 0.0008 | - | - | 0.6408 | 0.0000 | 0.0006 | 0.5001 | 0.0003 | 0.5001 | 0.9999 | 0.5001 | 0.1940 | 0.0003 | 0.0003 | 0.5001 |
| H2O | | 0.0000 | 0.1934 | 0.0000 | 0.0000 | - | - | 0.0000 | 1.0000 | 0.0000 | 0.4989 | 0.0000 | 0.4989 | 0.0000 | 0.4989 | 0.1934 | 0.0000 | 0.0000 | 0.4989 |
| CO | | 0.0000 | 0.0092 | 0.0065 | 0.0000 | - | - | 0.0037 | 0.0000 | 0.0065 | 0.0000 | 0.0150 | 0.0000 | 0.0000 | 0.0000 | 0.0092 | 0.0150 | 0.0150 | 0.0000 |
| Mass Flows | kg/hr | 19 461.39 | 22 575.85 | 22 575.85 | 19 461.39 | 17 015.03 | 2 384.18 | 62.18 | 6 962.51 | 22 575.85 | 19 397.90 | 3 177.96 | 19 397.90 | 12 373.21 | 19 397.90 | 22 575.85 | 63.56 | 3 114.40 | 19 397.90 |
| CO2 | kg/hr | 17 035.22 | 251.85 | 17 261.14 | 17 035.22 | 17 015.03 | - | 20.19 | 0.00 | 17 261.14 | 21.31 | 230.54 | 21.31 | 1.12 | 21.31 | 251.85 | 4.61 | 225.93 | 21.31 |
| H2 | kg/hr | 2 384.70 | 2 419.77 | 4 755.63 | 2 384.70 | - | 2 384.18 | 0.51 | 0.00 | 4 755.63 | 0.52 | 2 419.25 | 0.52 | 0.00 | 0.52 | 2 419.77 | 48.39 | 2 370.87 | 0.52 |
| CH3OH | kg/hr | 41.26 | 12 425.61 | 53.45 | 41.26 | - | - | 41.26 | 0.00 | 53.45 | 12 413.17 | 12.44 | 12 413.17 | 12 371.92 | 12 413.17 | 12 425.61 | 0.25 | 12.19 | 12 413.17 |
| H2O | kg/hr | 0.00 | 6 963.70 | 1.00 | 0.00 | - | - | 0.00 | 6 962.51 | 1.00 | 6 962.69 | 1.02 | 6 962.69 | 0.18 | 6 962.69 | 6 963.70 | 0.02 | 0.99 | 6 962.69 |
| CO | kg/hr | 0.21 | 514.93 | 504.63 | 0.21 | - | - | 0.21 | 0.00 | 504.63 | 0.21 | 514.71 | 0.21 | 0.00 | 0.21 | 514.93 | 10.29 | 504.42 | 0.21 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.8753 | 0.0112 | 0.7646 | 0.8753 | 1.0000 | - | 0.3248 | 0.0000 | 0.7646 | 0.0011 | 0.0725 | 0.0011 | 0.0001 | 0.0011 | 0.0112 | 0.0725 | 0.0725 | 0.0011 |
| H2 | | 0.1225 | 0.1072 | 0.2107 | 0.1225 | - | 1.0000 | 0.0083 | 0.0000 | 0.2107 | 0.0000 | 0.7613 | 0.0000 | 0.0000 | 0.0000 | 0.1072 | 0.7613 | 0.7613 | 0.0000 |
| CH3OH | | 0.0021 | 0.5504 | 0.0024 | 0.0021 | - | - | 0.6635 | 0.0000 | 0.0024 | 0.6399 | 0.0039 | 0.6399 | 0.9999 | 0.6399 | 0.5504 | 0.0039 | 0.0039 | 0.6399 |
| H2O | | 0.0000 | 0.3085 | 0.0000 | 0.0000 | - | - | 0.0000 | 1.0000 | 0.0000 | 0.3589 | 0.0003 | 0.3589 | 0.0000 | 0.3589 | 0.3085 | 0.0003 | 0.0003 | 0.3589 |
| CO | | 0.0000 | 0.0228 | 0.0224 | 0.0000 | - | - | 0.0034 | 0.0000 | 0.0224 | 0.0000 | 0.1620 | 0.0000 | 0.0000 | 0.0000 | 0.0228 | 0.1620 | 0.1620 | 0.0000 |
| Volume Flow | cum/hr | 614.14 | 323.39 | 920.25 | 48 824.98 | 9 536.54 | 855.23 | 67.10 | 7.53 | 1 211.75 | 23.08 | 301.10 | 22.29 | 16.18 | 22.29 | 822.38 | 6.02 | 295.07 | 23.02 |

*Table 24. Stream Summary for Configuration II "Methanol Synthesis with Two Reactors in Series" for catalyst "B".*

| | Units | CMAIN | F+R | FEEDCO2 | FEEDH2 | GAS | H2O | HLIGHT | HPROD | HPROD2 | LIGHT | LIGHT2 | MAIN | MCS4H | MEOH | OUTPUT | OUTPUT2 | PROD | PROD2 | PURGE | S2 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | | | |
| From | | TURBMAIN | MIX1 | | | CD | CD | HEAT1 | COOL1 | COOL3 | FLASH1 | FLASH2 | MIXMAIN | MCOMP | CD | FLASH1 | FLASH2 | R1 | R2 | B6 | HMAIN |
| To | | CD | MCOMP | MIX1 | MIX1 | B6 | | R2 | FLASH1 | FLASH2 | HEAT1 | B6 | HMAIN | R1 | | MIXMAIN | MIXMAIN | COOL1 | COOL3 | | TURBMAIN |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | - 454.24 | 8 592.05 | | - | | | | | | | | 6 185.66 | | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | | | |
| Phase | | Liquid Phase | Vapor Phase | Vapor Phase | Vapor Phas | Vapor Phas | Liquid Phas | Vapor Phase | | | Vapor Phas | Vapor Phase | | Vapor Phase | Liquid Phase | Liquid Phase | Liquid Phas | Vapor Phase | Vapor Phas | Vapor Phase | Liquid Phase |
| Temperature | C | 29.03 | 25.98 | 25.00 | 25.00 | 30.87 | 93.52 | 150.00 | 5.00 | 5.00 | 5.00 | 5.00 | 4.97 | 234.00 | 30.87 | 5.00 | 5.00 | 234.00 | 150.00 | 8.63 | 31.00 |
| Pressure | bar | 1.00 | 1.00 | 1.00 | 35.00 | 0.80 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 |
| Molar Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 0.628 | 0.973 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Molar Liquid Fraction | | 1.000 | - | - | - | - | 1.000 | - | 0.372 | 0.027 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Mass Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 0.152 | 0.719 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | - |
| Mass Liquid Fraction | | 1.000 | - | - | - | - | 1.000 | - | 0.848 | 0.281 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | 1.000 |
| Molar Enthalpy | kcal/mol | - 62.68 | - 13.39 | - 94.00 | 0.01 | - 56.47 | - 67.00 | - 0.01 | - 24.43 | - 1.74 | - 1.03 | - 0.13 | - 63.80 | - 11.82 | - 56.82 | - 63.94 | - 60.59 | - 18.74 | - 0.44 | - 0.18 | - 62.64 |
| Mass Enthalpy | kcal/kg | - 2 504.24 | - 1 673.45 | - 2 135.84 | 4.73 | - 1 895.26 | - 3 718.95 | - 3.77 | - 2 240.95 | - 634.73 | - 391.07 | - 66.45 | - 2 549.05 | - 1 477.54 | - 1 773.24 | - 2 572.24 | - 2 088.25 | - 1 719.16 | - 159.74 | - 90.02 | - 2 502.73 |
| Molar Entropy | cal/mol-K | - 47.24 | 0.96 | 0.69 | - 7.04 | - 5.52 | - 35.18 | - 6.15 | - 24.63 | - 10.90 | - 9.11 | - 9.64 | - 51.08 | - 4.31 | - 56.96 | - 50.83 | - 57.09 | - 10.56 | - 7.11 | 0.08 | - 47.12 |
| Mass Entropy | cal/gm-K | - 1.89 | 0.12 | 0.02 | - 3.49 | - 0.19 | - 1.95 | - 2.33 | - 2.26 | - 3.97 | - 3.45 | - 4.75 | - 2.04 | - 0.54 | - 1.78 | - 2.04 | - 1.97 | - 0.97 | - 2.59 | 0.04 | - 1.88 |
| Molar Density | mol/cc | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.03 | 0.00 | 0.02 | 0.04 | 0.03 | 0.00 | 0.00 | 0.00 | 0.03 |
| Mass Density | kg/cum | 844.05 | 0.32 | 1.78 | 2.79 | 0.94 | 925.12 | 7.18 | 66.06 | 11.43 | 10.72 | 8.25 | 870.26 | 18.23 | 785.95 | 872.43 | 832.41 | 25.94 | 7.47 | 0.07 | 841.85 |
| Enthalpy Flow | Gcal/hr | - 49.10 | - 36.83 | - 36.85 | 0.02 | - 0.06 | - 26.23 | - 0.01 | - 49.32 | - 2.12 | - 1.31 | - 0.16 | - 49.98 | - 32.52 | - 22.20 | - 48.01 | - 1.96 | - 37.84 | - 0.53 | - 0.22 | - 49.07 |
| Average MW | | 25.03 | 8.00 | 44.01 | 2.02 | 29.79 | 18.02 | 2.64 | 10.90 | 2.75 | 2.64 | 2.03 | 25.03 | 8.00 | 32.04 | 24.86 | 29.02 | 10.90 | 2.75 | 2.05 | 25.03 |
| Mole Flows | kmol/hr | 783.30 | 2 750.48 | 392.07 | 2 358.41 | 1.05 | 391.46 | 1 267.68 | 2 018.60 | 1 216.55 | 1 267.68 | 1 184.17 | 783.30 | 2 750.48 | 390.79 | 750.92 | 32.38 | 2 018.60 | 1 216.55 | 1 185.23 | 783.30 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0007 | 0.1425 | 1.0000 | - | 0.4546 | 0.0000 | 0.0054 | 0.0037 | 0.0000 | 0.0054 | 0.0000 | 0.0007 | 0.1425 | 0.0002 | 0.0007 | 0.0000 | 0.0037 | 0.0000 | 0.0004 | 0.0007 |
| H2 | | 0.0003 | 0.8575 | - | 1.0000 | 0.2552 | 0.0000 | 0.9795 | 0.6152 | 0.9730 | 0.9795 | 0.9995 | 0.0003 | 0.8575 | 0.0000 | 0.0003 | 0.0012 | 0.6152 | 0.9730 | 0.9989 | 0.0003 |
| CH3OH | | 0.4992 | - | - | - | 0.2840 | 0.0000 | 0.0003 | 0.1813 | 0.0213 | 0.0003 | 0.0004 | 0.4992 | - | 0.9997 | 0.4868 | 0.7857 | 0.1813 | 0.0213 | 0.0007 | 0.4992 |
| H2O | | 0.4998 | - | - | - | 0.0000 | 1.0000 | 0.0000 | 0.1906 | 0.0057 | 0.0000 | 0.0000 | 0.4998 | - | 0.0001 | 0.5122 | 0.2131 | 0.1906 | 0.0057 | 0.0000 | 0.4998 |
| CO | | 0.0000 | - | - | - | 0.0062 | 0.0000 | 0.0148 | 0.0093 | 0.0000 | 0.0148 | 0.0000 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0093 | 0.0000 | 0.0000 | 0.0000 |
| Mass Flows | kg/hr | 19 605.85 | 22 009.20 | 17 254.94 | 4 754.27 | 31.38 | 7 052.27 | 3 342.98 | 22 009.20 | 3 342.98 | 3 342.98 | 2 403.35 | 19 605.85 | 22 009.20 | 12 522.19 | 18 666.22 | 939.63 | 22 009.20 | 3 342.98 | 2 434.74 | 19 605.85 |
| CO2 | kg/hr | 24.32 | 17 254.94 | 17 254.94 | - | 21.07 | 0.00 | 302.39 | 326.71 | 0.11 | 302.39 | 0.11 | 24.32 | 17 254.94 | 3.25 | 24.32 | 0.00 | 326.71 | 0.11 | 21.18 | 24.32 |
| H2 | kg/hr | 0.54 | 4 754.27 | - | 4 754.27 | 0.54 | 0.00 | 2 503.02 | 2 503.48 | 2 386.11 | 2 503.02 | 2 386.04 | 0.54 | 4 754.27 | 0.00 | 0.46 | 0.08 | 2 503.48 | 2 386.11 | 2 386.58 | 0.54 |
| CH3OH | kg/hr | 12 528.05 | - | - | - | 9.59 | 0.00 | 12.69 | 11 725.50 | 831.74 | 12.69 | 16.50 | 12 528.05 | - | 12 518.46 | 11 712.81 | 815.24 | 11 725.50 | 831.74 | 26.08 | 12 528.05 |
| H2O | kg/hr | 7 052.76 | - | - | - | 0.00 | 7 052.27 | 1.07 | 6 929.52 | 124.81 | 1.07 | 0.50 | 7 052.76 | - | 0.49 | 6 928.45 | 124.31 | 6 929.52 | 124.81 | 0.50 | 7 052.76 |
| CO | kg/hr | 0.18 | - | - | - | 0.18 | 0.00 | 523.82 | 524.00 | 0.21 | 523.82 | 0.21 | 0.18 | - | 0.00 | 0.18 | 0.00 | 524.00 | 0.21 | 0.39 | 0.18 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0012 | 0.7840 | 1.0000 | - | 0.6715 | 0.0000 | 0.0905 | 0.0148 | 0.0000 | 0.0905 | 0.0000 | 0.0012 | 0.7840 | 0.0003 | 0.0013 | 0.0000 | 0.0148 | 0.0000 | 0.0087 | 0.0012 |
| H2 | | 0.0000 | 0.2160 | - | 1.0000 | 0.0173 | 0.0000 | 0.7487 | 0.1137 | 0.7138 | 0.7487 | 0.9928 | 0.0000 | 0.2160 | 0.0000 | 0.0000 | 0.0001 | 0.1137 | 0.7138 | 0.9802 | 0.0000 |
| CH3OH | | 0.6390 | - | - | - | 0.3055 | 0.0000 | 0.0038 | 0.5328 | 0.2488 | 0.0038 | 0.0069 | 0.6390 | - | 0.9997 | 0.6275 | 0.8676 | 0.5328 | 0.2488 | 0.0107 | 0.6390 |
| H2O | | 0.3597 | - | - | - | 0.0000 | 1.0000 | 0.0003 | 0.3148 | 0.0373 | 0.0003 | 0.0002 | 0.3597 | - | 0.0000 | 0.3712 | 0.1323 | 0.3148 | 0.0373 | 0.0002 | 0.3597 |
| CO | | 0.0000 | - | - | - | 0.0058 | 0.0000 | 0.1567 | 0.0238 | 0.0001 | 0.1567 | 0.0001 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0238 | 0.0001 | 0.0002 | 0.0000 |
| Volume Flow | cum/hr | 23.23 | 68 437.37 | 9 671.00 | 1 705.41 | 33.28 | 7.62 | 465.78 | 333.18 | 292.36 | 311.78 | 291.23 | 22.53 | 1 207.23 | 15.93 | 21.40 | 1.13 | 848.55 | 447.32 | 34 727.38 | 23.29 |

*Table 25. Stream Summary for Configuration III "Methanol Synthesis with Two Reactors in Series with a Recycle" for catalyst "B".*

| | Units | CMAIN | F+R | FEED | FEEDCO2 | FEEDH2 | GAS | H2O | HF+R | HLIGHT | HMAIN | HPROD | HPROD2 | LIGHT | LIGHT2 | MAIN | MCS4H | MEOH | OUTPUT | OUTPUT2 | PROD | PROD2 | PURGE | RECYCLE |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Description | | | | | | | | | | | | | | | | | | | | | | | | |
| From | | TURB3 | MIX2 | MIX1 | | | CD | CD | HEAT1 | HEAT2 | HEATMAIN | COOL1 | COOL3 | FLASH1 | FLASH2 | MIXMAIN | MCOMP | CD | FLASH1 | FLASH2 | R1 | R2 | MIX3 | MIX3 |
| To | | CD | HEAT1 | MCOMP | MIX1 | MIX1 | | | R1 | R2 | TURB3 | FLASH1 | FLASH2 | HEAT2 | MIX3 | HEATMAIN | MIX2 | | MIXMAIN | MIXMAIN | COOL1 | COOL3 | | MIX2 |
| Stream Class | | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN | CONVEN |
| Maximum Relative Error | | | | | | | | | | | | | | | | | | | | | | | | |
| Cost Flow | $/hr | | | | - 457.44 | 4 397.88 | | - | | | | | | | | | | 6 236.76 | | | | | | |
| MIXED Substream | | | | | | | | | | | | | | | | | | | | | | | | |
| Phase | | Liquid Phase | Vapor Phase | Vapor Phase | Vapor Phase | Vapor Phas | Vapor Phas | Liquid Phas | Vapor Phase | Vapor Phas | Liquid Phase | | | Vapor Phas | Vapor Phase | | Vapor Phase | Liquid Phase | Liquid Phase | Liquid Phas | Vapor Phase | Vapor Phas | Vapor Pha | Vapor Phas |
| Temperature | C | 23.27 | 109.84 | 25.76 | 25.00 | 25.00 | 34.71 | 93.52 | 240.00 | 180.00 | 25.00 | 5.00 | 5.00 | 5.00 | 5.00 | 4.95 | 177.70 | 34.71 | 5.00 | 5.00 | 240.00 | 180.00 | 5.00 | 5.00 |
| Pressure | bar | 1.00 | 100.00 | 1.00 | 1.00 | 35.00 | 0.80 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 0.80 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Molar Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 1.000 | - | 0.632 | 0.970 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | 1.000 |
| Molar Liquid Fraction | | 1.000 | - | - | - | - | - | 1.000 | - | - | 1.000 | 0.368 | 0.030 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | - |
| Mass Vapor Fraction | | - | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | - | 1.000 | 1.000 | - | 0.159 | 0.688 | 1.000 | 1.000 | 0.000 | 1.000 | - | - | - | 1.000 | 1.000 | 1.000 | 1.000 |
| Mass Liquid Fraction | | 1.000 | 0.000 | - | - | - | - | 1.000 | - | - | 1.000 | 0.841 | 0.312 | - | - | 1.000 | - | 1.000 | 1.000 | 1.000 | - | - | - | - |
| Molar Enthalpy | kcal/mol | - 62.79 | - 12.78 | - 23.16 | - 94.00 | 0.01 | - 53.66 | - 67.00 | - 11.79 | 0.14 | - 62.76 | - 24.25 | - 1.95 | - 1.09 | - 0.14 | - 63.80 | - 22.00 | - 56.73 | - 63.98 | - 60.13 | - 18.54 | - 0.39 | - 0.14 | - 0.14 |
| Mass Enthalpy | kcal/kg | - 2 508.52 | - 1 595.78 | - 1 872.89 | - 2 135.84 | 4.73 | - 1 844.98 | - 3 718.95 | - 1 471.80 | 51.13 | - 2 507.02 | - 2 233.55 | - 679.65 | - 401.23 | - 67.23 | - 2 548.54 | - 1 778.87 | - 1 770.43 | - 2 578.95 | - 2 031.26 | - 1 707.87 | - 134.92 | - 67.23 | - 67.23 |
| Molar Entropy | cal/mol-K | - 47.64 | - 6.46 | 1.32 | 0.69 | - 7.04 | - 7.21 | - 35.18 | - 4.22 | - 5.55 | - 47.51 | - 24.37 | - 11.09 | - 8.99 | - 9.64 | - 51.09 | - 4.77 | - 56.70 | - 50.76 | - 58.03 | - 10.28 | - 6.70 | - 9.64 | - 9.64 |
| Mass Entropy | cal/gm-K | - 1.90 | - 0.81 | 0.11 | 0.02 | - 3.49 | - 0.25 | - 1.95 | - 0.53 | - 2.04 | - 1.90 | - 2.24 | - 3.88 | - 3.30 | - 4.74 | - 2.04 | - 0.39 | - 1.77 | - 2.05 | - 1.96 | - 0.95 | - 2.34 | - 4.74 | - 4.74 |
| Molar Density | mol/cc | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.00 | 0.03 | 0.01 | 0.00 | 0.00 | 0.00 | 0.03 | 0.00 | 0.02 | 0.04 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 |
| Mass Density | kg/cum | 850.34 | 23.99 | 0.50 | 1.78 | 2.79 | 0.91 | 925.12 | 18.04 | 6.95 | 848.43 | 65.46 | 11.95 | 11.08 | 8.26 | 870.13 | 31.63 | 781.29 | 873.00 | 828.23 | 25.46 | 7.29 | 8.26 | 8.26 |
| Enthalpy Flow | Gcal/hr | - 49.57 | - 35.40 | - 37.10 | - 37.11 | 0.01 | - 0.06 | - 26.42 | - 32.65 | 0.18 | - 49.54 | - 49.55 | - 2.39 | - 1.41 | - 0.16 | - 50.36 | - 35.24 | - 22.35 | - 48.13 | - 2.23 | - 37.89 | - 0.47 | - 0.00 | - 0.16 |
| Average MW | | 25.03 | 8.01 | 12.37 | 44.01 | 2.02 | 29.09 | 18.02 | 8.01 | 2.73 | 25.03 | 10.86 | 2.86 | 2.73 | 2.03 | 25.03 | 12.37 | 32.04 | 24.81 | 29.60 | 10.86 | 2.86 | 2.03 | 2.03 |
| Mole Flows | kmol/hr | 789.44 | 2 770.20 | 1 601.99 | 394.83 | 1 207.16 | 1.09 | 394.34 | 2 770.20 | 1 290.77 | 789.44 | 2 043.15 | 1 229.15 | 1 290.77 | 1 192.09 | 789.44 | 1 601.99 | 394.01 | 752.38 | 37.06 | 2 043.15 | 1 229.15 | 23.84 | 1 168.25 |
| Mole Fractions | | | | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0006 | 0.1425 | 0.2465 | 1.0000 | - | 0.3944 | 0.0000 | 0.1425 | 0.0049 | 0.0006 | 0.0033 | - | 0.0049 | - | 0.0006 | 0.2465 | 0.0001 | 0.0006 | - | 0.0033 | - | - | - |
| H2 | | 0.0004 | 0.8573 | 0.7535 | - | 1.0000 | 0.2546 | 0.0000 | 0.8573 | 0.9757 | 0.0004 | 0.6165 | 0.9694 | 0.9757 | 0.9995 | 0.0004 | 0.7535 | 0.0000 | 0.0003 | 0.0014 | 0.6165 | 0.9694 | 0.9995 | 0.9995 |
| CH3OH | | 0.4995 | 0.0002 | - | - | - | 0.3434 | 0.0000 | 0.0002 | 0.0003 | 0.4995 | 0.1782 | 0.0254 | 0.0003 | 0.0005 | 0.4995 | - | 0.9998 | 0.4833 | 0.8275 | 0.1782 | 0.0254 | 0.0005 | 0.0005 |
| H2O | | 0.4995 | 0.0000 | - | - | - | 0.0000 | 1.0000 | 0.0000 | 0.0000 | 0.4995 | 0.1899 | 0.0052 | 0.0000 | 0.0000 | 0.4995 | - | 0.0000 | 0.5157 | 0.1710 | 0.1899 | 0.0052 | 0.0000 | 0.0000 |
| CO | | 0.0000 | 0.0000 | - | - | - | 0.0075 | 0.0000 | 0.0000 | 0.0190 | 0.0000 | 0.0120 | 0.0000 | 0.0190 | 0.0000 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0120 | 0.0000 | 0.0000 | 0.0000 |
| Mass Flows | kg/hr | 19 761.51 | 22 182.68 | 19 809.87 | 17 376.38 | 2 433.50 | 31.64 | 7 104.23 | 22 182.68 | 3 518.28 | 19 761.51 | 22 182.68 | 3 518.42 | 3 518.28 | 2 421.32 | 19 761.51 | 19 809.87 | 12 625.64 | 18 664.40 | 1 097.11 | 22 182.68 | 3 518.42 | 48.43 | 2 372.89 |
| CO2 | kg/hr | 21.48 | 17 376.38 | 17 376.38 | 17 376.38 | - | 18.88 | 0.00 | 17 376.38 | 277.19 | 21.48 | 298.67 | - | 277.19 | - | 21.48 | 17 376.38 | 2.59 | 21.48 | - | 298.67 | - | - | - |
| H2 | kg/hr | 0.56 | 4 787.23 | 2 433.50 | - | 2 433.50 | 0.56 | 0.00 | 4 787.23 | 2 538.88 | 0.56 | 2 539.34 | 2 401.95 | 2 538.88 | 2 401.85 | 0.56 | 2 433.50 | 0.00 | 0.45 | 0.11 | 2 539.34 | 2 401.95 | 48.04 | 2 353.81 |
| CH3OH | kg/hr | 12 635.02 | 17.05 | - | - | - | 11.97 | 0.00 | 17.05 | 12.90 | 12 635.02 | 11 665.13 | 1 000.18 | 12.90 | 17.39 | 12 635.02 | - | 12 623.04 | 11 652.22 | 982.79 | 11 665.13 | 1 000.18 | 0.35 | 17.04 |
| H2O | kg/hr | 7 104.23 | 0.41 | - | - | - | 0.00 | 7 104.22 | 0.41 | 1.10 | 7 104.23 | 6 991.11 | 114.62 | 1.10 | 0.41 | 7 104.23 | - | 0.01 | 6 990.02 | 114.21 | 6 991.11 | 114.62 | 0.01 | 0.41 |
| CO | kg/hr | 0.23 | 1.63 | - | - | - | 0.23 | 0.00 | 1.63 | 688.21 | 0.23 | 688.44 | 1.67 | 688.21 | 1.67 | 0.23 | - | 0.00 | 0.23 | 0.00 | 688.44 | 1.67 | 0.03 | 1.63 |
| Mass Fractions | | | | | | | | | | | | | | | | | | | | | | | | |
| CO2 | | 0.0011 | 0.7833 | 0.8772 | 1.0000 | - | 0.5968 | 0.0000 | 0.7833 | 0.0788 | 0.0011 | 0.0135 | - | 0.0788 | - | 0.0011 | 0.8772 | 0.0002 | 0.0012 | - | 0.0135 | - | - | - |
| H2 | | 0.0000 | 0.2158 | 0.1228 | - | 1.0000 | 0.0176 | 0.0000 | 0.2158 | 0.7216 | 0.0000 | 0.1145 | 0.6827 | 0.7216 | 0.9920 | 0.0000 | 0.1228 | 0.0000 | 0.0000 | 0.0001 | 0.1145 | 0.6827 | 0.9920 | 0.9920 |
| CH3OH | | 0.6394 | 0.0008 | - | - | - | 0.3783 | 0.0000 | 0.0008 | 0.0037 | 0.6394 | 0.5259 | 0.2843 | 0.0037 | 0.0072 | 0.6394 | - | 0.9998 | 0.6243 | 0.8958 | 0.5259 | 0.2843 | 0.0072 | 0.0072 |
| H2O | | 0.3595 | 0.0000 | - | - | - | 0.0000 | 1.0000 | 0.0000 | 0.0003 | 0.3595 | 0.3152 | 0.0326 | 0.0003 | 0.0002 | 0.3595 | - | 0.0000 | 0.3745 | 0.1041 | 0.3152 | 0.0326 | 0.0002 | 0.0002 |
| CO | | 0.0000 | 0.0001 | - | - | - | 0.0073 | 0.0000 | 0.0001 | 0.1956 | 0.0000 | 0.0310 | 0.0005 | 0.1956 | 0.0007 | 0.0000 | - | 0.0000 | 0.0000 | 0.0000 | 0.0310 | 0.0005 | 0.0007 | 0.0007 |
| Volume Flow | cum/hr | 23.24 | 924.67 | 39 821.50 | 9 739.07 | 872.92 | 34.81 | 7.68 | 1 229.83 | 506.51 | 23.29 | 338.87 | 294.50 | 317.49 | 293.18 | 22.71 | 626.26 | 16.16 | 21.38 | 1.32 | 871.37 | 482.84 | 5.86 | 287.31 |

# Appendix D – Heat Integration

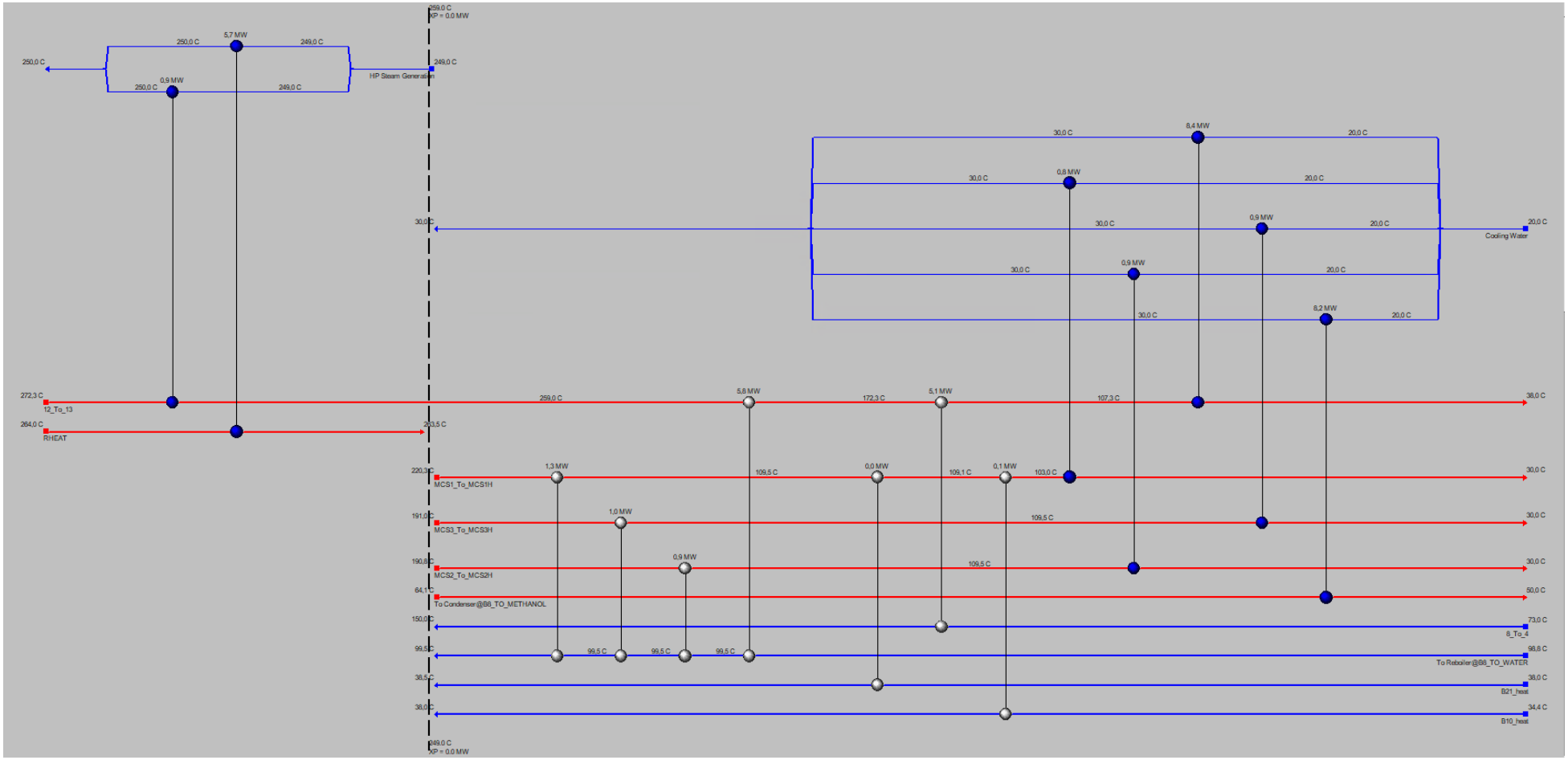


*Figure 10. Heat integration for the "Conventional Process" in Aspen Energy Analyzer.*

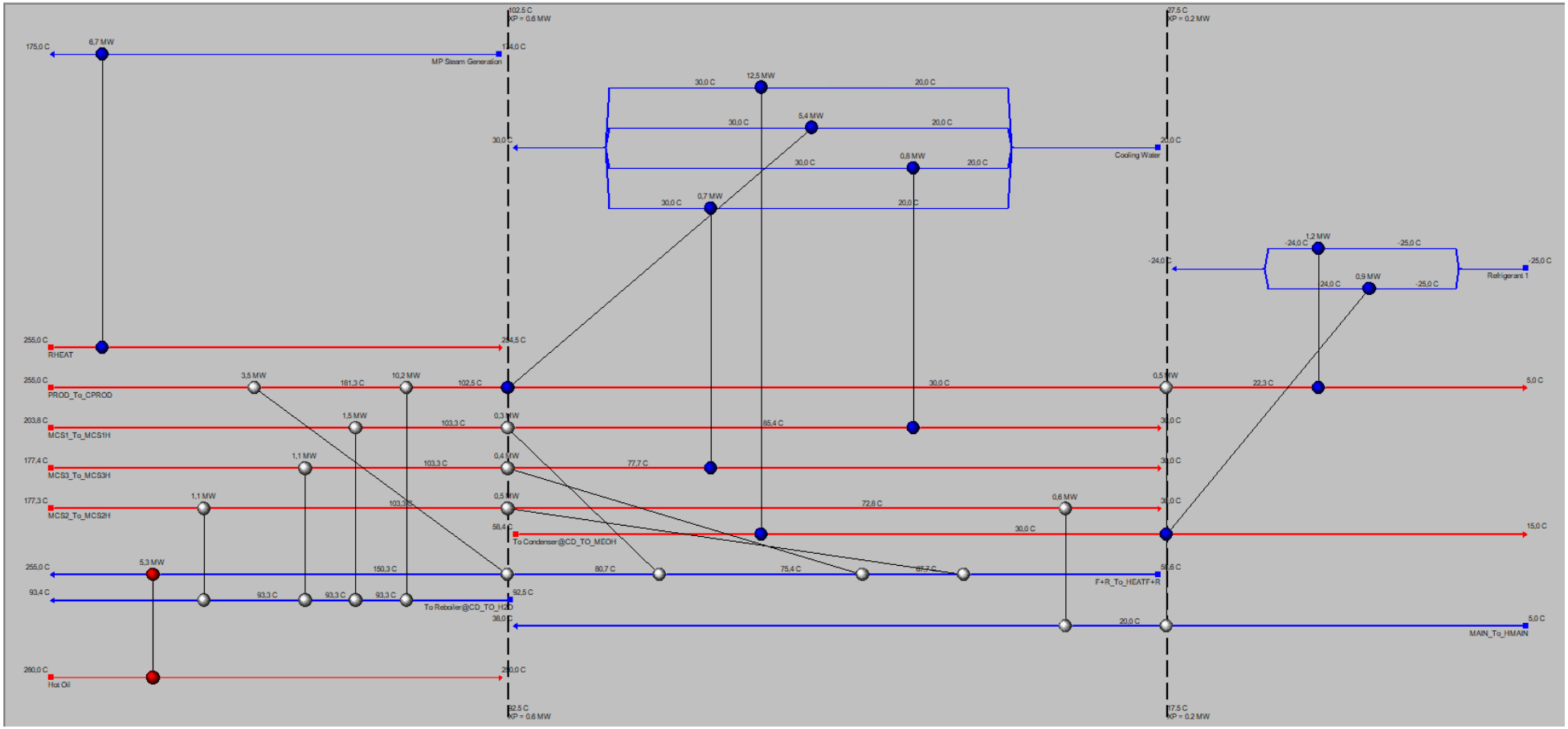


*Figure 11. Heat integration for Configuration I "Methanol Synthesis with a Recycle" for catalyst "A" in Aspen Energy Analyzer.*

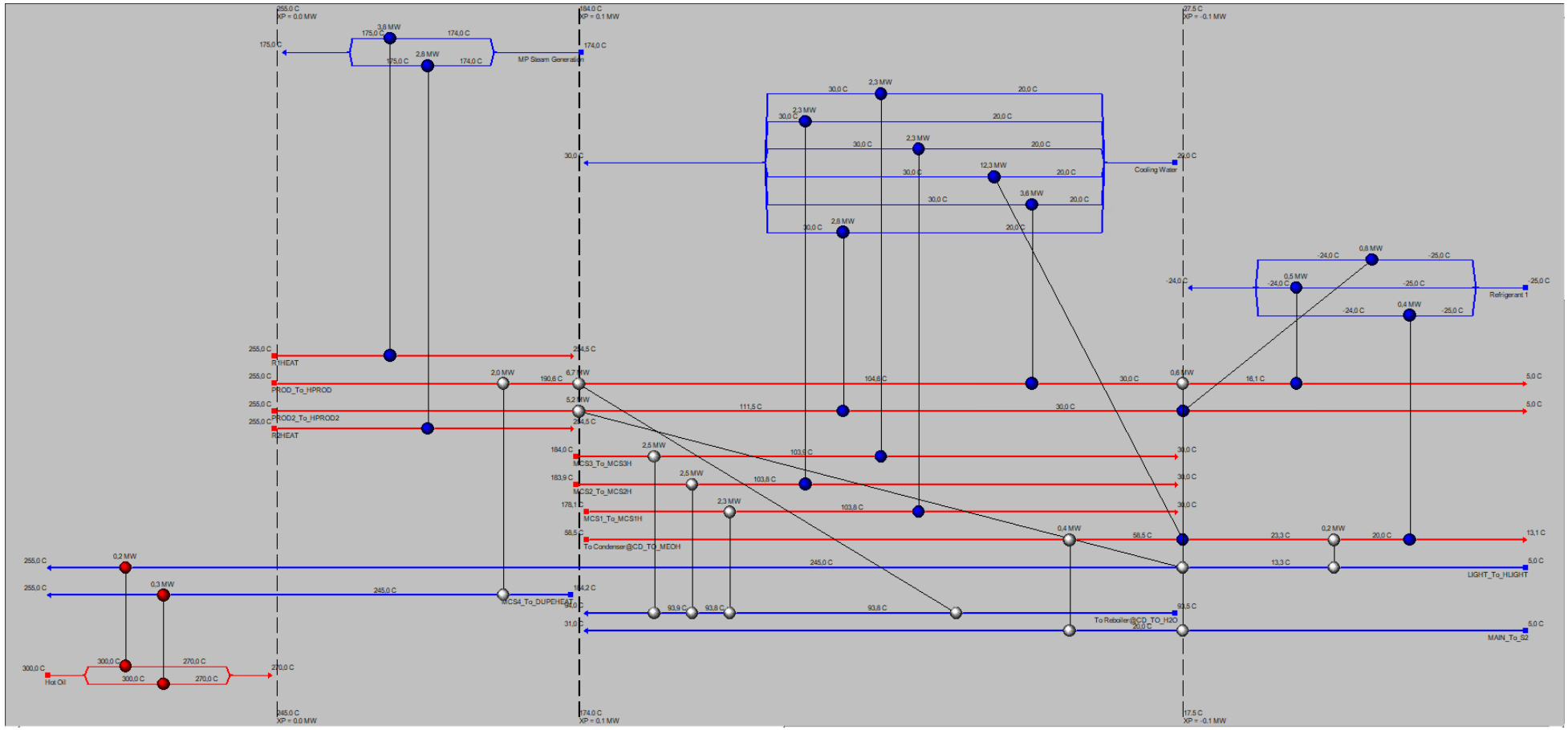


*Figure 12. Heat integration for Configuration II "Methanol Synthesis with Two Reactors in Series" for catalyst "A" in Aspen Energy Analyzer.*

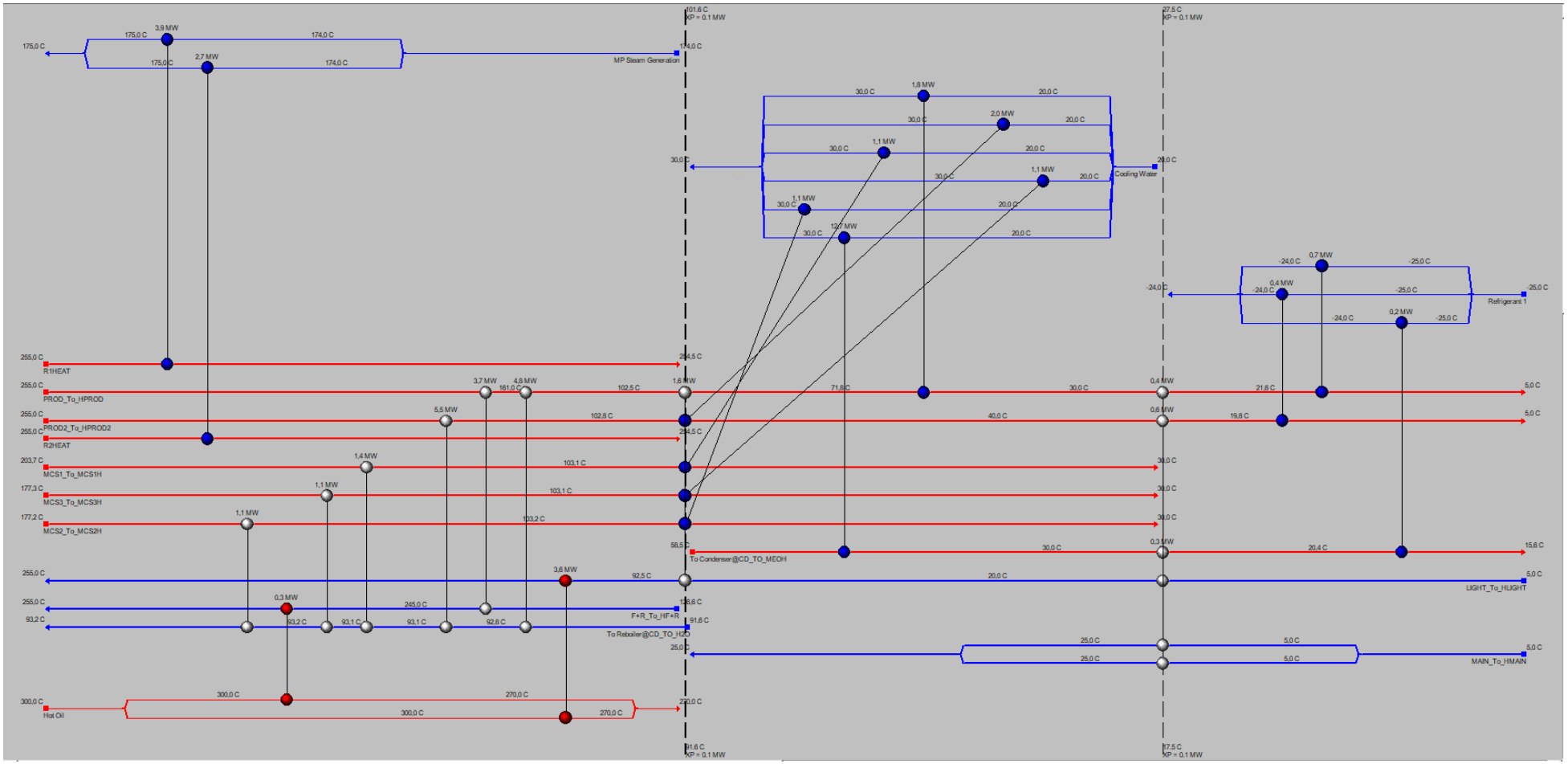


*Figure 13. Heat integration for Configuration III "Methanol Synthesis with Two Reactors in Series with a Recycle" for catalyst "A" in Aspen Energy Analyzer.*

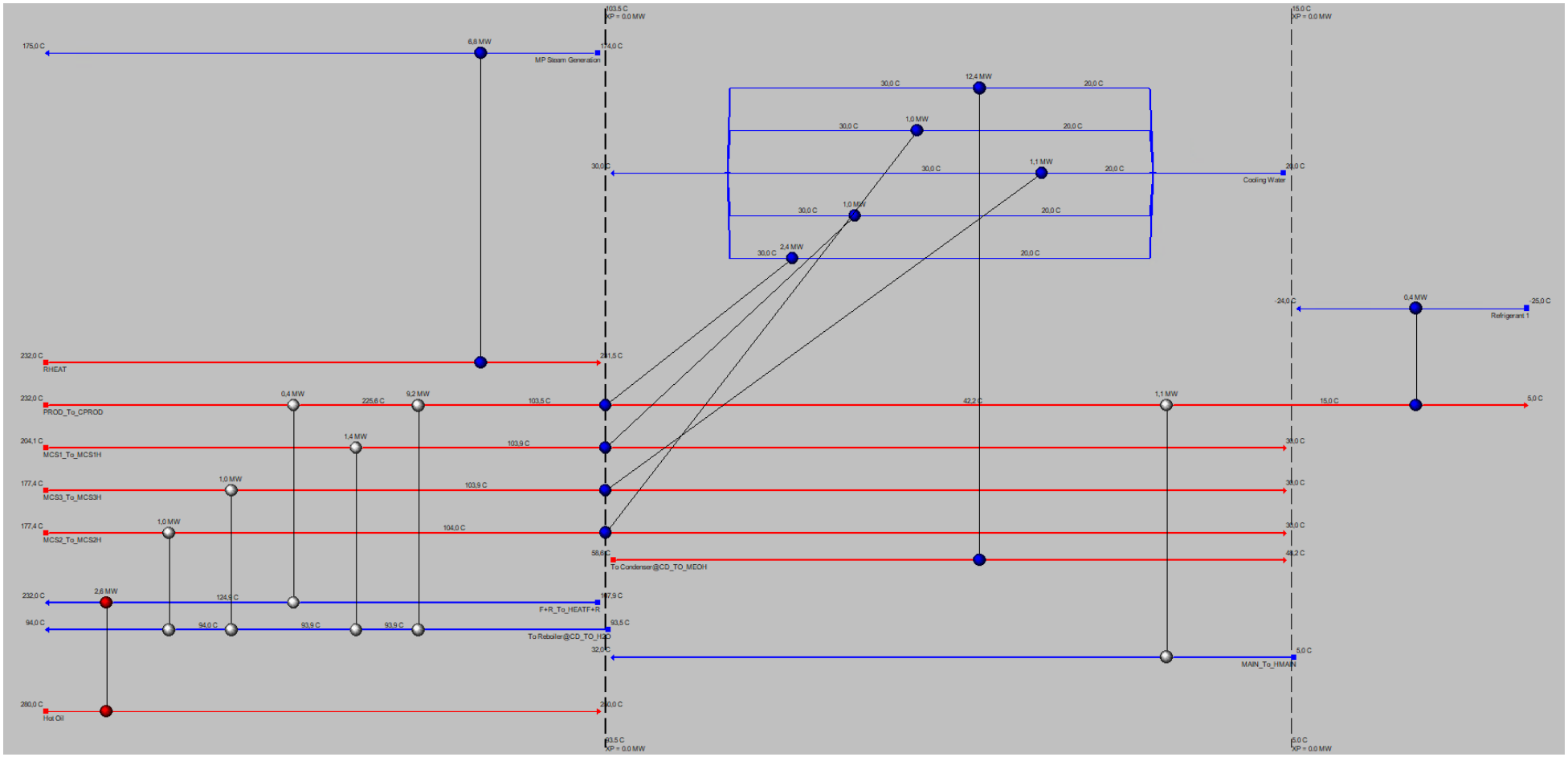


*Figure 14. Heat integration for Configuration I "Methanol Synthesis with a Recycle" for catalyst "B" in Aspen Energy Analyzer.*

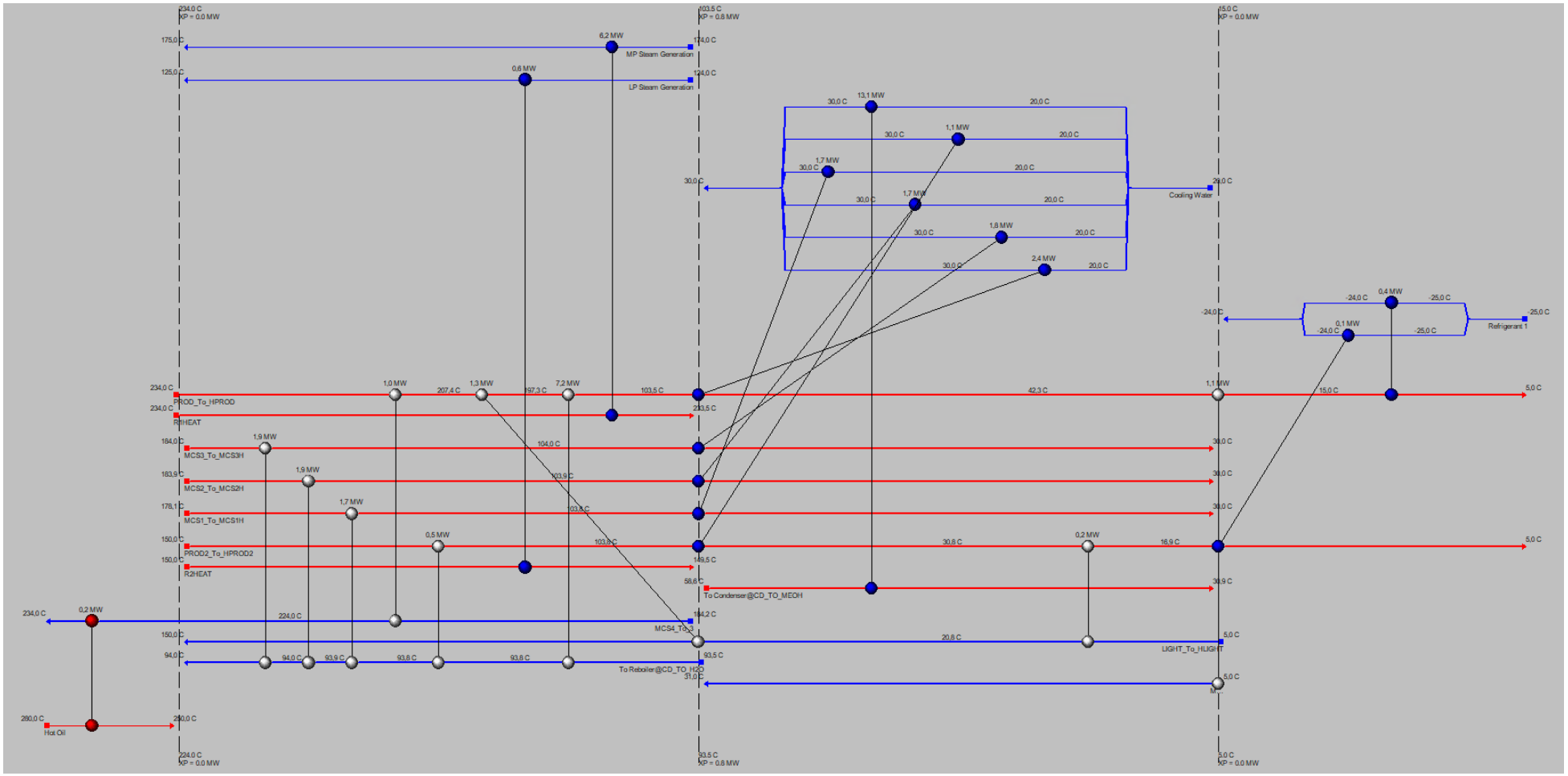


*Figure 15. Heat integration for Configuration II "Methanol Synthesis with Two Reactors in Series" for catalyst "B" in Aspen Energy Analyzer.*

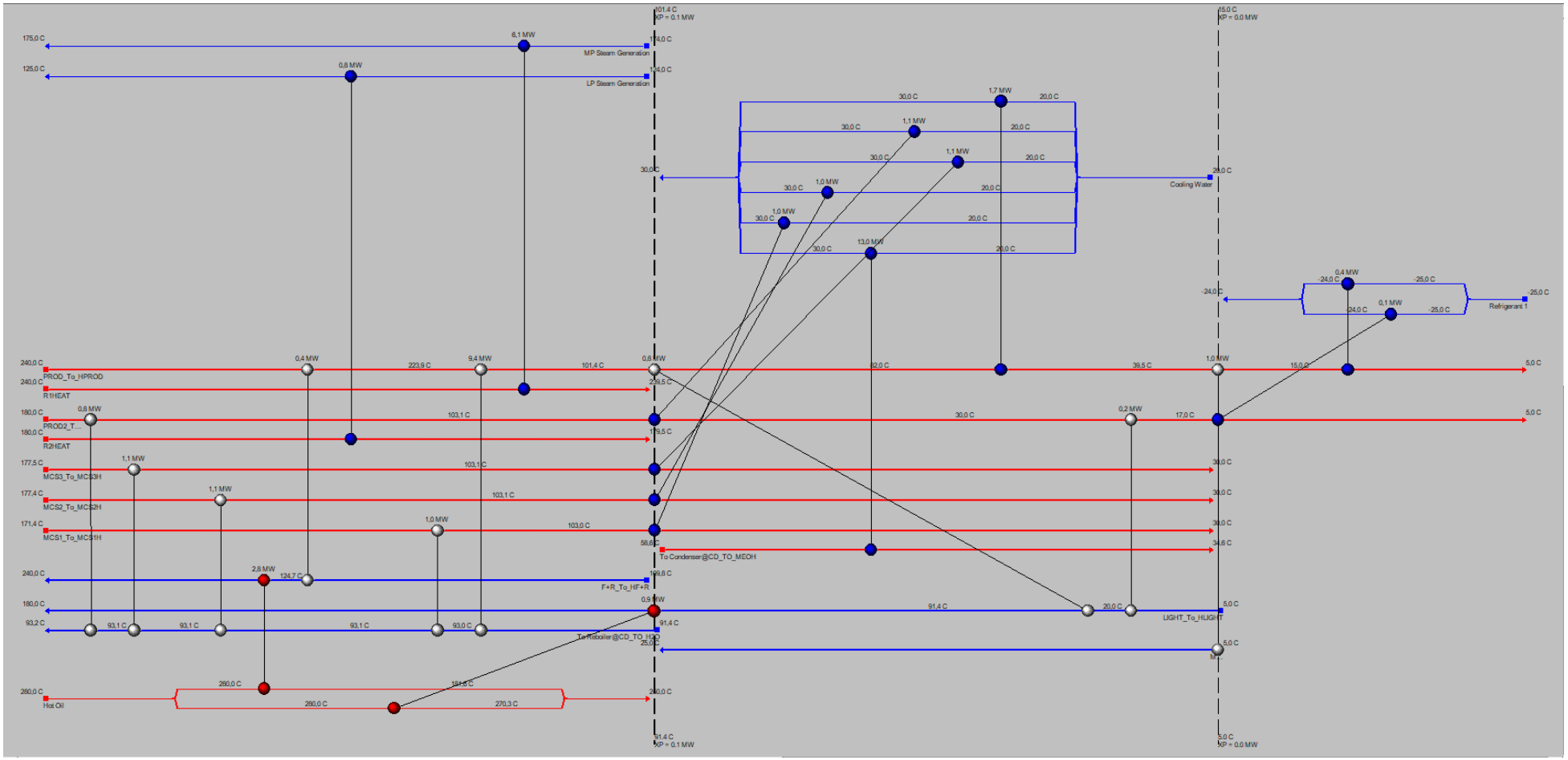


*Figure 16. Heat integration for Configuration III "Methanol Synthesis with Two Reactors in Series with a Recycle" for catalyst "B" in Aspen Energy Analyzer.*