C.1 Gas to Liquid Process

Index

Introduction

Chemical looping partial oxidation processes, including gasification and reforming, provide multiple synthesis pathways for the production of various chemicals. The gas to liquids process is a process that converts natural gas to syngas, which is then used for the synthesis of transportation fuels such as gasoline, kerosene, and diesel. The specifics of the process are discussed in Section 6.2.2. Using the appropriate operating conditions, syngas from partial oxidation chemical looping can be tailored to produce a syngas composition that is compatible for liquid fuels production via the Fischer-Tropsch reaction. An iron-titanium complex metal oxide (ITCMO) is used as the oxygen carrier. The details of syngas generation using ITCMO for liquid fuels production is discussed in Section 6.6.

Process Configuration

The schematic for the Gas to liquid (GTL) process is shown in Figure C.1.1. Natural gas, simplified to methane, is obtained at a delivery pressure of 30 bar. The natural gas is first heated to 600 °C and then subjected to a Joule-Thomson expansion to a pressure slightly greater than the reducer reactor operating pressure. This expander is coupled with the compressor for syngas to reduce the overall syngas compression energy requirement. Specifically, the syngas produced in the reducer reactor is compressed using a compressor that is coupled with the expander, in what is known as a turbo-expander. The methane inlet stream must first be heated prior to expansion to compensate for the decrease in temperature that occurs during adiabatic expansion.

The air inlet stream is compressed using a compressor with interstage cooling. The air stream is pre-heated to 600 °C using heat from the syngas exiting the reducer reactor, which is cooled to 150 °C. The gas exiting the combustor, oxygen depleted air, is then cooled using two heat-extraction passes. The first pass cools the oxygen depleted air stream to 400 °C and the secondary pass further reduces the temperature to 170 °C. After being cooled to 150 °C, the syngas stream enters a condenser to remove the water. The water-free syngas stream is then compressed using the turbo-expander coupled with a compressor and a standalone syngas compressor.

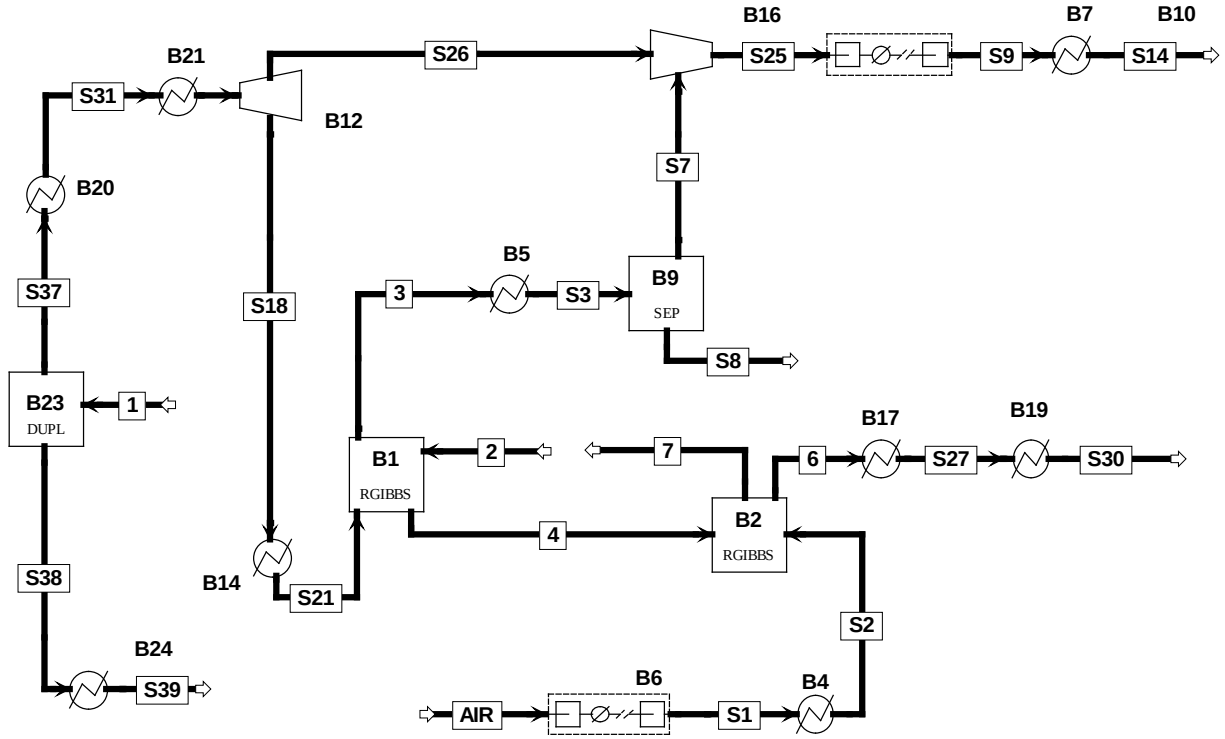

Figure C.1.1 Process simulation of Gas to Liquids Process

Components and Physical Properties

The process simulation is completed using Aspen Plus® simulation software. This section lists the definitions and settings used for process modeling. The parameters used in this Gas to Liquid simulation are defined in Table C.1 and Table C.2.

Table C.1 Parameters used in the simulation

Parameter	Setting
Stream Class	MIXCISLD
Thermodynamic and Physical data bank (in order)	INORGANIC, PURE32, AQUEOUS, SOLIDS
Method filter	SYNFUEL
Base Method	RKS-BM
Reactor module type	RGIBBS

Table C.2 List of components

Type: Solid	
Hematite (Fe_2O_3)	Iron-dialuminum tetraoxide ($FeAl_2O_4$)
Magnetite (Fe_3O_4)	Titanium dioxide: Rutile (TiO_2)
Wuestite ($Fe_{0.947}O$)	Iron-titanium trioxide: Ilmenite ($FeTiO_3$)
Iron (Fe)	Silicon carbide (SiC)
Aluminum oxide: alpha-Corundum (Al_2O_3)	Carbon (C)
Type: Conventional	
Methane (CH_4)	Water (H_2O)
Carbon monoxide (CO)	Oxygen (O_2)
Carbon dioxide (CO_2)	Nitrogen (N_2)
Hydrogen (H_2)	

Operating Conditions

Parameters for the inlet streams and reactors are given in Table C.3 and Table C.4, respectively. Some values in the tables are calculated based on user input.

Table C.3 Inlet stream specifications

Stream	CH_4	Air	Fe_2O_3	TiO_2
Flow Rate (kmol/hr)	1	3.3	1.224	7.542
Temperature (°C)	38	25	1,190	1,190
Pressure (bar)	29.6	1	5	5

Table C.4 Chemical looping reactor operating conditions

Block	Reducer	Combustor
Temperature (°C)	910	1,190
Pressure (bar)	5	5

Results and Discussion

Table C.5 provides the molar flow rates of each component for each stream based on the parameters given in Tables C.1 through C.4. Table C.6 provides a break-down of the available heat within the chemical looping block. The stream numbers and unit operation name correspond to those in the Gas to Liquid Aspen Plus simulation file.

Table C.5 Flow rate of chemical looping reforming species

Stream	1	2	3	4	6	7	AIR
Flow rate (kmol/hr)							
CO	0	0	0.888	0	0	0	0
CO2	0	0	0.073	0	0	0	0
H2	0	0	1.731	0	0	0	0
H2O	0	0	0.19	0	0	0	0
CH4	1	0	0.039	0	0	0	0
C	0	0	0	0	0	0	0
FE2O3	0	1.224	0	0	0	1.224	0
FE3O4	0	0	0	0	0	0	0
FE0.947O	0	0	0	0	0	0	0
FE	0	0	0	0	0	0	0
AL2O3	0	0	0	0	0	0	0
FEAL2O4	0	0	0	0	0	0	0
SIC	0	0	0	0	0	0	0
O2	0	0	0	0	0.011	0	0.623
N2	0	0	0	0	2.677	0	2.677
TIO2	0	7.542	0	5.094	0	7.542	0
FETIO3	0	0	0	2.448	0	0	0
Total Mole Flow (kmol/hr)	1	8.767	2.922	7.542	2.688	8.767	3.3
Mass Flow (kg/hr)	16.043	797.97	35.63	778.383	75.34	797.97	94.927
Temperature (°C)	38	1190	909.9	909.9	1,190	1,190	25
Pressure (bar)	29.6	5	5	5	5	5	1

Table C.6 Available heat from various streams

Unit	Description	Q (cal/sec)	Tin (°C)	Tout (°C)	P (bar)
B17 (S36)	spent air	3,902	1,190	398	5
B2	combustor	563	1,190	1,190	5

Conclusions

The Gas to Liquids process using chemical looping natural gas reforming is simulated in Aspen Plus®. Natural gas, simplified to methane, is partially oxidized in the reducer reactor by the ITCMO particles to produce high purity syngas. The syngas generated in this process has a H_2:CO ratio around 2, which is suitable for Fischer-Tropsch synthesis to produce liquid fuels. The chemical looping reforming system is operated at 5 bar, which significantly reduces the compression energy compared to ambient pressure.

Appendix

The Aspen Plus file of the STS-GTL process is given in the file titled, “C.1 Gas to Liquid.”