Design of Shift Reactor unit to Convert CO to CO_2

Vishnu Mamidi, Dinesh Malakala, Manuel Mammen, Deepak Kumar, Siva Kumar and C RaviKumar

Department of Chemical Engineering,

Visvesvaraya National Institute of Technology, Nagpur

Introduction:

The water gas shift reaction is used to produce hydrogen for syngas, comprises of CO_2 and H_2. This process can also be used for producing combustion gas with lower levels of carbon from a carbon-rich syngas. The shift reaction is mildly exothermic and equilibrium limited. Therefore, the extent of reaction becomes limited as the temperature increases along the length of the reactor. A two-stage process with inter-stage cooling is used to achieve the desired extent of conversion. A higher temperature results in a higher reaction rate, and a chromia-promoted iron oxide catalyst is used in the first stage. The second stage operates at a comparatively lower temperature, where a copper-zinc catalyst is used.

$$\mathrm{CO} + \mathrm{H_2O} \leftrightarrow \mathrm{CO_2} + \mathrm{H_2} \qquad \Delta H = -41\ KJ\ mol^{-1}.$$

Description:

Feed – Carbon monoxide

It is a colorless, odorless, and tasteless gas that is slightly less dense than air. It is toxic to hemoglobic animals (both invertebrate and vertebrate, including humans) when encountered in concentrations above about 35 ppm. It has wide range of industrial applications and especially in the manufacturing of aldehydes

Product – Carbon di Oxide

In the chemical industry, carbon dioxide is mainly consumed as an ingredient in the production of urea, with a smaller fraction being used to produce methanol and a range of other products, such as metal carbonates and bicarbonates. Some carboxylic acid derivatives such as sodium salicylate are prepared using CO_2 by the Kolbe-Schmitt reaction.

In addition to conventional processes using CO_2 for chemical production, electrochemical methods are also being explored at a research level. In particular, the use of renewable energy for production of fuels from CO_2 (such as methanol) is attractive as this could result in fuels that could be easily transported and used within conventional combustion technologies but have no net CO_2 emissions

Catalyst – Iron oxide and Zinc

The catalyst used in shift reactions are iron oxide and zinc. The former is used in the high Temperature Reactor with catalyst loading of 1121 kg/metre cube and zinc catalyst in low temperature reactor with a loading of 1442 kg/metre cube.

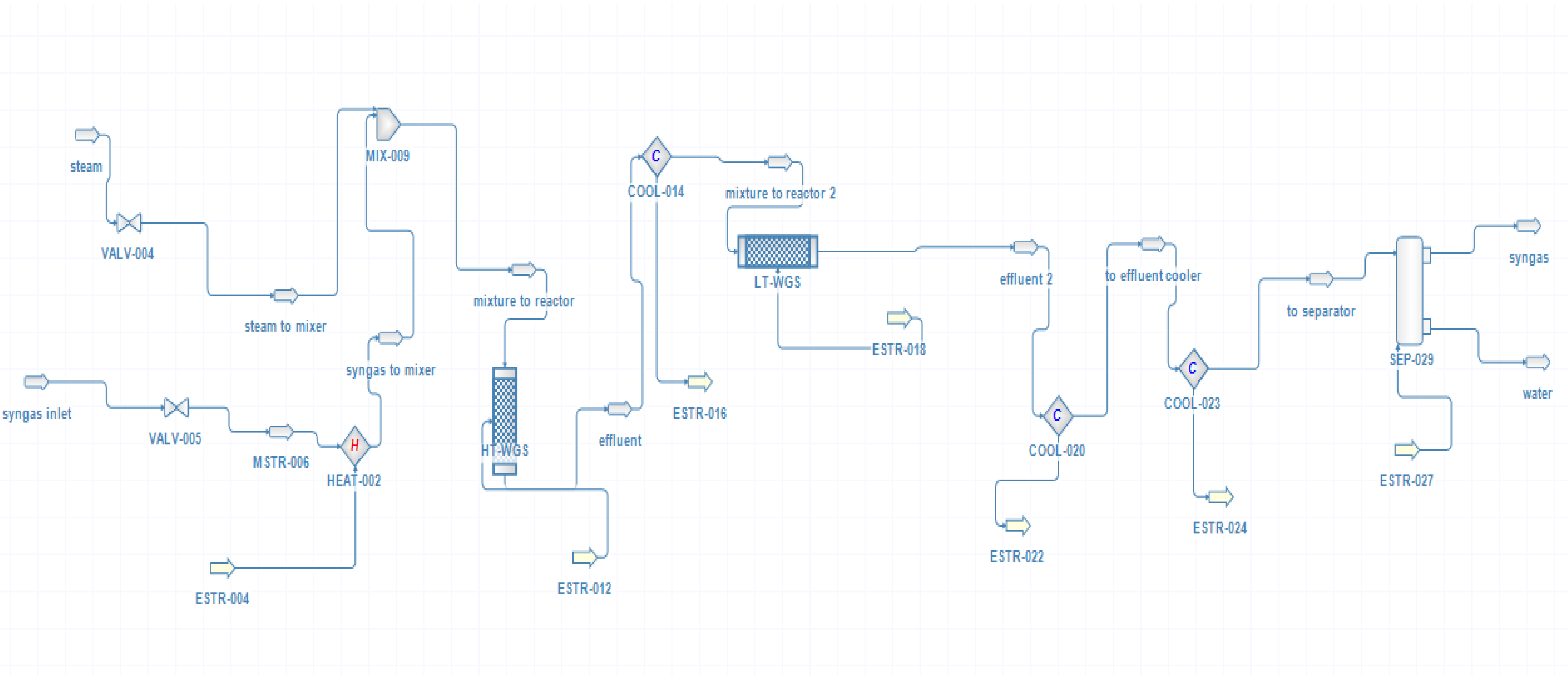

Fig. 1: Flow sheet made in DWSIM for the shift reactor.

Process

In the given process first we take 93 moles of steam and 31 moles of carbon monoxide so that it is in the ratio of 3:1 for achieving 90% conversion. We heat the syngas stream and mix with incoming steam stream in a mixer and send the mixture to HTWGS reactor with iron oxide catalyst as loading. The effluent from this reactor is cooled and we send it to LTWGS with zinc catalyst as loading. We then cool the effluent from the second reactor and send it to a flash separator to separate water and enriched syngas.

Reaction Kinetics:

$$K_{eq} = e^{-4.33+\frac{4577.9}{T}}$$

For 589K < T < 756K

$$K_{eq} = e^{-4.72+\frac{4800}{T}}$$

For 422K < T < 589K

Particle density = 2018 kg/m^3 for iron catalyst

= 2483 kg/m^3 for copper-zinc catalyst

Bulk density = 1121 kg/m^3 for the first bed with iron catalyst

= 1442 kg/m^3 for copper-zinc catalyst

Particle diameter = 1.0 mm for both catalysts

Simulation and Conclusion

The above process was modelled and simulated in DWSIM software.

The results obtained after simulation and calculations are found to be consistent with the results in reference with appendix B12 of with reference from appendix B12 of the, Richard Turton et al. (2009). *Analysis, Synthesis and design of Chemical processes.* Prentice Hall; 3rd edition.

Summary Table

Stream	Syngas	Syngas to mixer	Steam	Mixture to reactor	
Temperature	115	320	325	320.1491	C
Pressure	16.5	15.2	16.2	15.2	bar
Mass Flow	2,191.23	2,191.23	1,679.00	3,870.22	kg/h
Molar Flow	100	100	93.2	193.2	kmol/h
Vapor Phase Molar Fraction	1	1	1	1	

Table 1: Properties of inlet streams

Stream	Effluent	Effluent 2	Syngas	Water	
Temperature	320.1383	203.071412	132	132	C
Pressure	15.17193	14.198753	12.79875	12.79875	bar
Mass Flow	3,870.22	3,870.22	2,708.16	1,162.06	kg/h
Molar Flow	193.2	193.2	128.73	64.47001	kmol/h
Vapor Phase Molar Fraction	1	1	1	0	

References:

Richard Turton et al. (2009). *Analysis, Synthesis and design of Chemical processes.* Prentice Hall; 3rd edition.