Chapter 4

Process modelling using Aspen Plus software

Refer again to figure 3.2 for the following discussion.

4.1 The natural gas feedstock

A typical natural gas composition was used for all the simulations. The methane content is that of high quality natural gas (see table 4.1).

Table 4.1: Natural gas composition for GTL study

Component	Mole %
CH_4	94.8%
C_2H_6	2.6%
C_3H_8	0.2%
C_4H_{10}	0.03%
C_5H_{12}	0.01%
C_6H_{14}	0.01%
N_2	1.6%
CO_2	0.81%
O_2	0.02%

This composition is common to the natural gas found in the Union Gas system in North America (Union-Gas, May 2002).

4.2 The reformer

The autothermal reformer is modelled by the Gibbs reactor model in Aspen Plus. This reactor model calculates the product compositions from the reactor by minimising the total free Gibbs energy. The reforming (refer to equations 2.1 and 2.2) as well as the water gas shift reaction (refer to equation 2.3) are thus taken into account, without specifying the necessary reaction equations. Therefore there is no need to change the reformer model if a separation change is made in the light oil and water distillation column. This is very handy for when the recycle loop is closed and the range of hydrocarbons being reformed changes with every iteration. The reformer pressure was specified at 24 bar and the temperature was varied between 850°C and 1170°C to find the optimum temperature to satisfy the design goals.

4.3 Feed preheater

The feed preheater supplies the maximum preheating to the hydrocarbon feed. The stream is heated from 160°C to $(T_{ref} - 75)$°C. The two stream heat exchanger model was used in Aspen Plus with a design constraint on the outlet temperature of the cold stream at $(T_{ref} - 75)$°C. It was assumed that the high preheat temperatures would not cause soot formation or metal dusting in the heat exchanger.

4.4 The steam generator

The steam generator is also modelled with the two stream heat exchanger model in Aspen Plus. Saturated water at 24 bar are heated to superheated steam by the reformer tailgas. The design constraint of 430°C was put on the cold stream outlet temperature. This results in saturated water being heated from 222°C to 430°C which is superheated steam at the correct temperature and pressure for feed to the reformer.

The saturated water is obtained from environmental water (pumped to 24 bar) which has been saturated with heat from the exothermic Fischer–Tropsch reaction. Depending on the temperature of the reformer, extra superheated steam needs to be imported for feed to the reformer or surplus superheated steam can be exported. The exported steam is converted to electricity in a steam turbine and used in the GTL process for pumps and blowers.

4.5   Water separation

Although cooling of the syngas has already taken place with the two heat exchangers, further cooling to 50°C is done to condense out any excess water which could deactivate the cobalt catalyst in the Fischer–Tropsch reactor. The syngas is then heated again to 260°C (with imported heat) to minimise any exergy losses in the FT reactor because of mixing irreversibilities.

4.6   The low temperature Fischer-Tropsch reactor

The slurry phase Fischer-Tropsch reactor (rstoic) was modelled according to the reactions taking place in the reactor with the assumption that olefin production will not be modelled. The alkane reactions for the production of C_1 to C_{24} were modelled by the 'rstoic' model in Aspen Plus. The reaction modelled for these components was the following:

$$nCO + (2n + 1)H_2 \rightarrow C_nH_{2n+2} + nH_2O \tag{4.1}$$
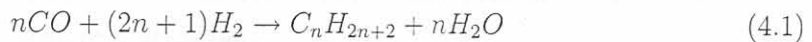
The conversion of each of these reactions were calculated according to the Anderson-Schulz-Flory distribution. For this distribution, the probability of chain growth is given. See also chapter 2. This probability is a value between 0 and 1. The higher the value, the higher the probability of high carbon chain growth and thus more waxes. For this simulation a CO conversion of 80% was assumed (Espinoza *et al.*, 1999). The reactor temperature and pressure were 260°C and 23 bar. A pressure decrease of 1 bar was assumed. The Fischer–Tropsch reactions are very exothermic. Cooling is done by water at 24 bar in a cooling coil inside the reactor. The water is then saturated and used as feed for the steam generator.

4.7   The separation column

The separation column (Sep block) was modelled as a simplification of both the heavy oil separation drum and the light oil and water distillation column. This was done as to minimise convergence problems with separation as the composition of the recycle changes with every iteration.

With the separation block it was assumed that all water could be removed from the light gases exiting the separation column. The other assumptions were that all methane

could be separated and recycled into the loop.

4.8 The condenser (modelled separate because of the Sep block)

The condenser was modelled as a cooler to cool the product gas from the separation column to 40 °C as would have automatically happened if the light oil and distillation column would have been modelled with the Radfrac model. This must be done for the exergy analysis, because the purge stream has to be at the lowest possible temperature.

4.9 The blower

The blower was modelled by the Aspen Plus compressor model with a specified discharge pressure. The tailgas is compressed to 26 bar to reduce any pressure exergy losses when mixing occurs with the fresh feed at 26 bar.

4.10 The purge

A split block introduced the purge stream. Depending on the temperature of the reformer, the purge was always varied to obtain maximum recycling for the syngas to the Fischer–Tropsch reactor to reach a $H_2:CO$ ratio of 2.15. As already mentioned, this specific ratio is necessary to stay in a specific product range in the Fischer–Tropsch reactor.

The purged stream has high heating value and can therefore be converted to electricity to maintain a high exergetic efficiency for the whole process. This is done by a combined cycle. With the combined cycle the purge gas is incinerated in a gas turbine, and steam is generated from the hot gas turbine exhaust gases for additional electricity generation in a steam turbine. The combined cycle has an exergy efficiency of 50%.