1.Gasification

Drying (RStoic) reactor specification

Temperature (°C)	100
Pressure (bar)	1
Fractional conversion	0.325 component of pyrolysis-oil

Decomposition (Ryield) reactor specification

Temperature (°C)	500
Pressure (bar)	1
Yield options	Component yields
H_2	4.15
C	32.8
O_2	30.4
N_2	0.27
S	0.001

Combustion and gasification (RGibbs) reactor specification

Calculation option	Calculate phase equilibrium and chemical equilibrium
Temperature (°C)	800
Pressure (bar)	1
Products	Identity possible products
Component	Valid phases
CO	Mixed
H_2	Mixed
CO_2	Mixed
CH_4	Mixed
NH_3	Mixed
H_2S	Mixed

2. Rectisol

Rectisol (RadFrac) block specification

Configuration:

Calculation type	Equilibrium
Number of stages	15
Condenser	none
Reboiler	none
Valid phases	Vapor- Liquid
convergence	Standard

Steams:

Feed streams

Name	Stage	Convention
9	1	Above-stage
10	15	On-stage

Product streams

Name	Stage	Phase	Basis	Units
11	15	Liquid	Mole	kmol/hr
12	1	Vapor	Mole	kmol/hr

Pressure:

View	Top/Bottom
Top stage/ Condenser pressure (bar)	1~80

3. Methanol synthesis

Methanol synthesis (RPLUG) reactor specifications:

Reaction type:	Reactor with specified temperature
Configuration:	
Multitube reactor:	Number of tubes: 11458
Tube dimensions:	Length: 12.0 meter Diameter: 0.03675 meter
Catalyst specifications:	
Bed voidage	0.5
Particle density	2000 kg/m^3

Kinetic LHHW Parameters

R1 ($CO_2 + H_2 \rightarrow CO + H_2O$)	
Kinetic factor	k = 1 n = 0 E = 0 kJ/kmol
Driving-force expressions (partial pressure):	
Term 1	
Concentration exponents for reactants	CO_2 = 1, H_2 = 0
Concentration exponents for products	CO = 0, H_2O = 0
Coefficients:	A = 4.80, B = -11398.2, C = 0, D = 0
Term 2	
Concentration exponents for reactants	CO_2 = 0, H_2 = -1
Concentration exponents for products	CO = 1, H_2O = 1
Coefficients:	A = 0.13, B = -6624.98, C = 0, D = 0

Adsorption expression:	
Adsorption term exponent :	1
Concentration exponents:	
Term 1:	$H_2 = 0$, $H_2O = 0$
Term 2:	$H_2 = -1$, $H_2O = 1$
Term 3:	$H_2 = 0.5$, $H_2O = 0$
Term 4:	$H_2 = 0$, $H_2O = 1$
Adsorption constants:	
Term 1:	A = 0, B = 0, C = 0, D = 0
Term 2:	A = 8.15, B =0, C = 0, D = 0
Term 3:	A = -6.45, B =2068.44, C = 0, D = 0
Term 4:	A = -34.95, B =14928.90, C = 0, D = 0

R2 ($CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$)	
Kinetic factor	k = 1 n = 0 E = 0 kJ/kmol
Driving-force expressions (partial pressure)	
Term1	
Concentration exponents for reactants	$CO_2 = 1$, $H_2 = 1$
Concentration exponents for products	$CH_3OH = 0$, $H_2O = 0$
Coefficients:	A = -29.87, B = 4413.76, C = 0, D = 0
Term 2:	
Concentration exponents for reactants	$CO_2 = 0$, $H_2 = -2$
Concentration exponents for products	$CH_3OH = 1$, $H_2O = 1$
Coefficients:	A=17.55, B = -2645.97, C = 0, D = 0
Adsorption expression	
Adsorption term exponent :	3
Concentration exponents:	
Term 1:	$H_2 = 0$, $H_2O = 0$
Term 2:	$H_2 = -1$, $H_2O = 1$
Term 3:	$H_2 = 0.5$, $H_2O = 0$
Term 4:	$H_2 = 0$, $H_2O = 1$
Adsorption constants:	
Term 1:	A = 0, B = 0, C = 0, D = 0
Term 2:	A = 8.15, B =0, C = 0, D = 0
Term 3:	A = -6.45, B =2068.44, C = 0, D = 0
Term 4:	A = -34.95, B =14928.9, C = 0, D = 0