Methanol Synthesis

- Physical Property - Analysis Tools - Binary Analysis
- Adding Reactions(Equilibrium//Kinetic)
- Operations - Isothermal Reactor - Recycling // Purging
- Keq - Given // Calculated
- Units - R-CST // Distal // DSTWU// RadFrac // Compressor
- Results - Customize // Export // Plot

Problem Statement

- Methanol is to be synthetized from Syngas
- Reactor is ISOTHERMAL

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H = -91 kJ/mol$$
$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H = -49.5 kJ/mol$$
$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H = -41.2 kJ/mol$$

  - Equilibrium Data (see in simulation)
- Feed:
  - CO, CO2, H2 → 50,200, 600
  - T = 50°C, P = 1 bar

Objectives

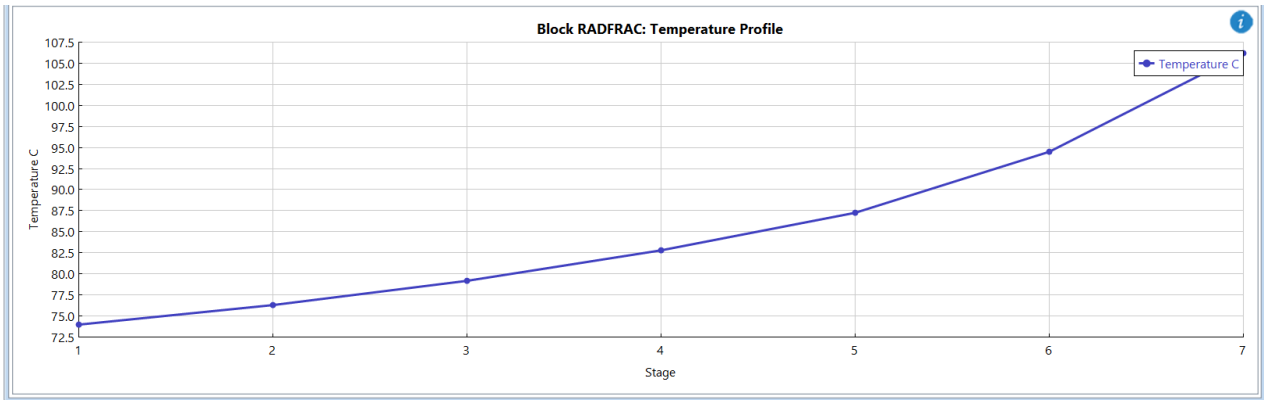
- Main goal is to:
  - Pre-heat feed (to T = 270°C, P = 40 bar)
  - Add Recycle + Feed to the Reactor Inlet
  - Cool down (50°C, P = 10 bar)
  - Separate Vapors from products
  - Re-heat recycle (T = 270°C, P = 40 bar)
  - PURGE gas
  - Drop pressure of liquid product
  - Separate methanol/water

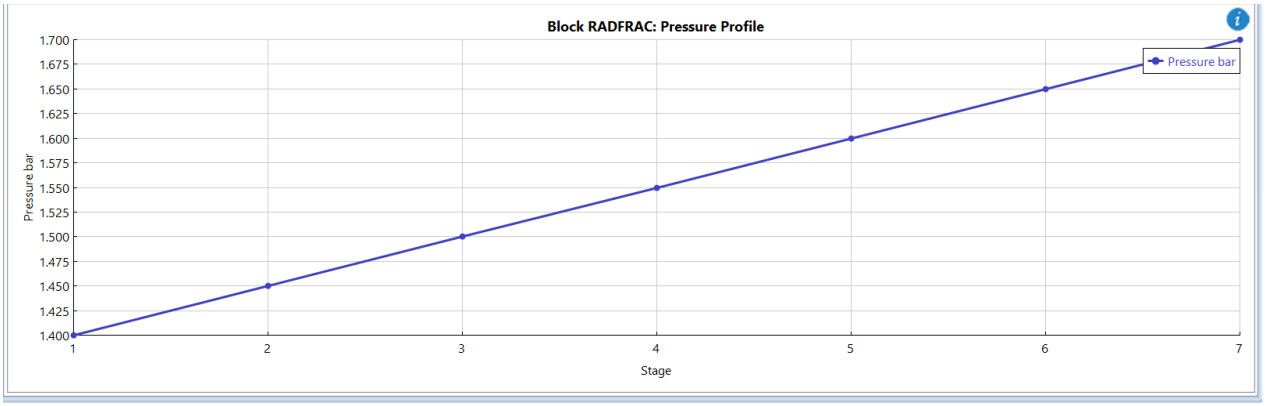
Design Methodology

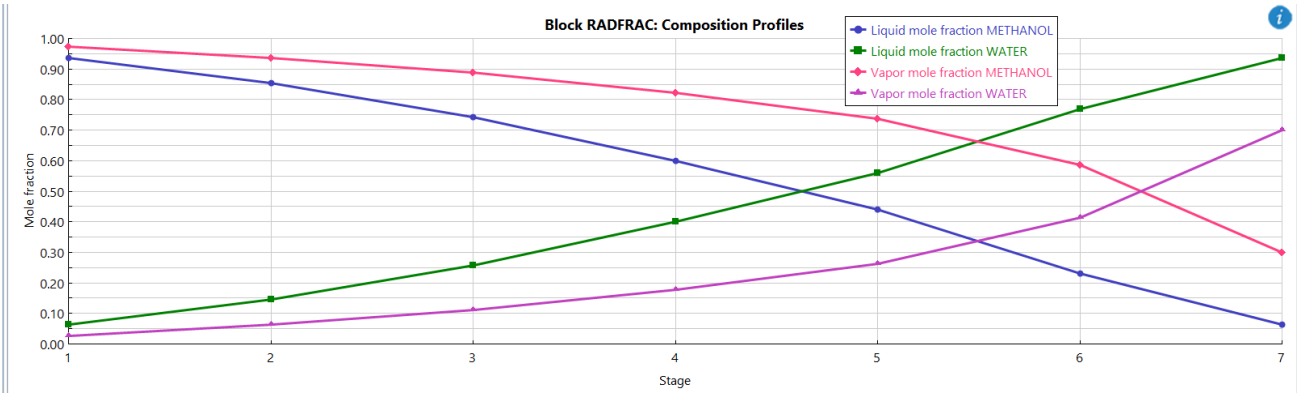
- (Ai) Verify Heat duty of Reactor (pre/after recycle)
- (Aii) For the CSTR, verify Calculated Keq vs. Given Built-in Expressions
- (B) Purge Ratio vs. Recycle
- (C) Use Binary Analysis for Distillation
- (D) DSWTU No. recommended Stages, given RR = 1.5
- (E) DSWTU → DISTL → RadFrac
- (F) Reboiler/Condenser Heating Duties of Column
- (G) Final Product Purity Specification

Final Product Purity Specification

DISTL						Radfrac				
Mole Flows	kmol/hr	399.759856	199.8803039	199.8795522		Mole Flows	kmol/hr	199.879928	199.879928	49.76021869
CO	kmol/hr	0	0	0		CO	kmol/hr	0	0	49.28029359
CO2	kmol/hr	0	0	0		CO2	kmol/hr	0	0	0.4799251018
H2	kmol/hr	0	0	0		H2	kmol/hr	0	0	0
METHANOL	kmol/hr	200.2397812	11.06129599	189.1784852		METHANOL	kmol/hr	187.3597366	12.88004456	0
WATER	kmol/hr	199.5200748	188.8190079	10.70106695		WATER	kmol/hr	12.52019139	186.9998835	0
Mole Fractions						Mole Fractions				
CO		0	0	0		CO		0	0	0.9903552453
CO2		0	0	0		CO2		0	0	0.00964475467
H2		0	0	0		H2		0	0	0
METHANOL		0.5009001734	0.05533970368	0.9464606431		METHANOL		0.9373614374	0.06443890936	0
WATER		0.4990998266	0.9446621768	0.05353747648		WATER		0.06263856264	0.9355610906	0


Block RADFRAC: Temperature Profile
Temperature C
Temperature C
107.5
105.0
102.5
100.0
97.5
95.0
92.5
90.0
87.5
85.0
82.5
80.0
77.5
75.0
72.5
1
2
3
4
5
6
7
Stage


Block RADFRAC: Pressure Profile
Pressure bar
Pressure bar
1.700
1.675
1.650
1.625
1.600
1.575
1.550
1.525
1.500
1.475
1.450
1.425
1.400
1
2
3
4
5
6
7
Stage


Block RADFRAC: Composition Profiles
Liquid mole fraction METHANOL
Liquid mole fraction WATER
Vapor mole fraction METHANOL
Vapor mole fraction WATER
Mole fraction
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
1
2
3
4
5
6
7
Stage