PART 1: Reactors in Series

This part is about simulation of ammonia production plant. The process of ammonia production depends on several basic parts:

1. Hydrogen production (steam reforming)
2. Nitrogen addition (air reforming)
3. Carbon monoxide and carbon dioxide removal
4. Ammonia production

These basic parts are described based on several conditions mentioned in **TWO** different questions. Select only **ONE** question and simulate the process.

QUESTION 1 (50 marks; CLO4, PLO5, C3 – Application; WP1, WP4; WK3, WK4, WK5, WK6)

Hydrogen Production:

Hydrogen is predominantly generated from the reaction amongst methane and steam. Natural gas is sent to the primary reformer for steam reforming, where the superheated steam is fed into the reformer with the methane at 639.7 ^oC in the presence of a nickel catalyst where methane is converted to hydrogen, carbon dioxide and small amounts of carbon monoxide.

$$CH_4 + 2H_2O \xrightarrow{50\ \%} CO_2 + 4H_2 \quad (1)$$

$$CH_4 + H_2O \xrightarrow{20\ \%} CO + 3H_2 \quad (2)$$

Nitrogen addition:

The synthesis gas from the primary reformer is sent to the secondary reformer where syngas blended with air within the sight of profoundly exothermic reaction amongst oxygen and methane produces more hydrogen. In this secondary reformer, nitrogen is added as air is added to the reformer.

$$2CH_4 + O_2 \xrightarrow{10\ \%} 2CO + 4H_2 \quad (3)$$

$$CH_4 + O_2 \xrightarrow{20\ \%} CO_2 + 2H_2 \quad (4)$$

Carbon monoxide removal:

It is important to reduce the carbon monoxide as lower as possible in order to avoid toxin to the ammonia production. At high temperature shift conversion (HTSC), carbon monoxide is converted to carbon dioxide at 583 °C and likewise carbon monoxide is expelled and changed over to carbon dioxide at low temperature shift conversion (LTSC) around 325 °C.

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (5)$$

Ammonia production:

Ammonia is produced due to reaction between hydrogen and nitrogen.

$$N_2 + 3H_2 \xrightarrow{80\ \%} 2NH_3 \quad (6)$$

In this simulation, Peng-Robinson fluid package is used.

a) Building up the simulation basic (15 marks)

- How many components required in this simulation? List all of them.

(3 marks)

- Define the Reaction Set-1 for Reactions (1) and (2). Screenshot these reactions (Rxn-1, Rxn-2) and Reaction Set-1.

(3 marks)

- Define the Reaction Set-2 for Reactions (3) and (4). Screenshot these reactions (Rxn-3, Rxn-4) and Reaction Set-2.

(3 marks)

- Define Rxn-5 for Reaction (5). Screenshot this reaction.

(3 marks)

- Define Rxn-6 for Reaction (6). Screenshot this reaction.

(3 marks)

b) Steam and air reforming process analysis (15 marks)

- Install a conversion reactor as Primary Reformer with Methane stream (F = 1000 kmol/h, T = 371 °C, P = 3345 kPa) and Steam stream (F = 3000 kmol/h, T = 639.7 °C, P = 3345 kPa). Name the top stream as “To Secondary Reformer”. Screenshot the reactor. Calculate the percentage conversion of methane.

(8 marks)

- Install a conversion reactor as Secondary Reformer with Air stream (F = 500 kmol/h, T = 30 °C, P = 3445 kPa). Name the top stream as "To HTSC". Screenshot the "To HTSC" composition in molar flowrate. Identify the molar flowrate of hydrogen.

(7 marks)

c) Water Gas Shift process analysis (15 marks)

- Make sure the temperature of "To HTSC" is set at 583 °C before entering equilibrium reactor of HTSC. Name the top stream as "To LTSC". Screenshot the "To LTSC" composition in molar flowrate. Identify the molar flowrate of carbon monoxide. Compare the molar flowrate of hydrogen now with the one in (1b)?

(8 marks)

- Make sure the temperature of "To LTSC" is set at 325 °C before entering equilibrium reactor of LTSC. Name the top stream as "To Ammonia Reactor". Screenshot the "To Ammonia Reactor" composition in molar flowrate. Compare the molar flowrate of hydrogen now with the one previously.

(7 marks)

d) Ammonia production analysis (5 marks)

- Install a conversion reactor as Ammonia Reactor. Screenshot all the components in molar flowrate.

(5 marks)

QUESTION 2 (50 marks; CLO4, PLO5, C3 – Application; WP1, WP4; WK3, WK4, WK5, WK6)

Hydrogen Production:

Hydrogen is predominantly generated from the reaction amongst methane and steam. Natural gas is sent to the primary reformer for steam reforming, where the superheated steam is fed into the reformer with the methane at 609.7 °C in the presence of a nickel catalyst where methane is converted to hydrogen, carbon dioxide and little amounts of carbon monoxide.

$$CH_4 + 2H_2O \xrightarrow{40\ \%} CO_2 + 4H_2 \quad (7)$$

$$CH_4 + H_2O \xrightarrow{30\ \%} CO + 3H_2 \quad (8)$$

Nitrogen addition:

The synthesis gas from the primary reformer is sent to the secondary reformer where syngas blended with air within the sight of profoundly exothermic reaction amongst oxygen and methane produces more hydrogen. In this secondary reformer, nitrogen is added as air is added to the reformer.

$$2CH_4 + O_2 \xrightarrow{10\ \%} 2CO + 4H_2 \quad (9)$$

$$CH_4 + O_2 \xrightarrow{20\ \%} CO_2 + 2H_2 \quad (10)$$

Carbon monoxide removal:

It is important to reduce the carbon monoxide as lower as possible in order to avoid toxin to the ammonia production. At high temperature shift conversion (HTSC), carbon monoxide is converted to carbon dioxide at 553 °C and likewise carbon monoxide is expelled and changed over to carbon dioxide at low temperature shift conversion (LTSC) around 305 °C.

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (11)$$

Ammonia production:

Ammonia is produced due to reaction between hydrogen and nitrogen.

$$N_2 + 3H_2 \xrightarrow{80\,\%} 2NH_3 \qquad (12)$$

In this simulation, Peng-Robinson fluid package is used.

a) Building up the simulation basic (15 marks)

- How many components required in this simulation? List all of them.

(3 marks)

- Define the Reaction Set-1 for Reactions (1) and (2). Screenshot these reactions (Rxn-1, Rxn-2) and Reaction Set-1.

(3 marks)

- Define the Reaction Set-2 for Reactions (3) and (4). Screenshot these reactions (Rxn-3, Rxn-4) and Reaction Set-2.

(3 marks)

- Define Rxn-5 for Reaction (5). Screenshot this reaction.

(3 marks)

- Define Rxn-6 for Reaction (6). Screenshot this reaction.

(3 marks)

b) Steam and air reforming process analysis (15 marks)

- Install a conversion reactor as Primary Reformer with Methane stream (F = 1000 kmol/h, T = 371 ^oC, P = 3345 kPa) and Steam stream (F = 3000 kmol/h, T = 609.7 ^oC, P = 3345 kPa). Name the top stream as "To Secondary Reformer". Screenshot the reactor. Calculate the percentage conversion of methane.

(8 marks)

- Install a conversion reactor as Secondary Reformer with Air stream (F = 700 kmol/h, T = 30 ^oC, P = 3445 kPa). Name the top stream as "To HTSC". Screenshot the "To HTSC" composition in molar flowrate. Identify the molar flowrate of hydrogen.

(7 marks)

c) Water Gas Shift process analysis (15 marks)

- Make sure the temperature of "To HTSC" is set at 553 ^oC before entering equilibrium reactor of HTSC. Name the top stream as "To LTSC". Screenshot the "To LTSC" composition in molar flowrate. Identify the molar flowrate of carbon monoxide. Compare the molar flowrate of hydrogen now with the one in (1b)?

(8 marks)

- Make sure the temperature of "To LTSC" is set at 305 ^{o}C before entering equilibrium reactor of LTSC. Name the top stream as "To Ammonia Reactor". Screenshot the "To Ammonia Reactor" composition in molar flowrate. Compare the molar flowrate of hydrogen now with the one previously.

(7 marks)

d) Ammonia production analysis (5 marks)

- Install a conversion reactor as Ammonia Reactor. Screenshot all the components in molar flowrate.

(5 marks)

PART 2: Separators in Series

This part is about simulation of a sequence of distillation columns which is described based on several conditions mentioned in **TWO** different questions. Select only **ONE** question and simulate the process.

QUESTION 1 (50 marks; CLO1, PLO2, C4 – Analysis; WP1, WP4; WK3, WK4, WK5, WK6)

In this simulation, use Chao-Seader fluid package. Based on information given in Table 1, answer all the following questions.

Table 1: Feed stream information

Feed Components	**Composition**	**Desired Purity (%)**
Cyclopentane	0.1	99.0
Benzene	0.5	
Toluene	0.2	
Ethylbenzene	0.1	
Dicyclopentadiene	0.1	
Pressure (kPa)	101.3	
Feed condition	Saturated Liquid	
Flowrate (kmol/h)	1000	

b) Building up the simulation basic (10 marks)

- Based on information given, list all four variables defined for this case.

  (3 marks)

- What is the dew/boiling point temperature of this mixture?

  (2 marks)

- Briefly explain how to make this mixture in a vapour phase?

  (3 marks)

- What is the boiling temperature of this mixture? Screenshot the feed information.

  (2 marks)

b) Distillation columns sequence analysis (12 marks)

- Define a direct sequence.

(3 marks)

- Manually draw the direct sequence for this Feed by showing corresponding component at all product streams.

(3 marks)

- Define an indirect sequence.

(3 marks)

- Manually draw the indirect sequence for this Feed by showing corresponding component at all product streams.

(3 marks)

c) Distillation columns sequence simulation analysis (14 marks)

- Simulate the direct sequence in (b) using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this direct sequence.

(2 marks)

- Simulate the indirect sequence in (b) using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this indirect sequence.

(2 marks)

d) Driving force distillation columns sequence analysis (14 marks)

- Develop and plot the driving force curves for this Feed.

(5 marks)

- Synthesize and manually draw this sequence by showing corresponding component at all product streams.

(2 marks)

- Simulate this sequence using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this sequence.

(2 marks)

QUESTION 2 (50 marks; CLO1, PLO2, C4 – Analysis; WP1, WP4; WK3, WK4, WK5, WK6)

In this simulation, use Peng Robinson fluid package. Based on information given in Table 2, answer all the following questions.

Table 2: Feed stream information

Feed Components	Composition	Desired Purity (%)
Benzene	0.1	
Methylcyclohexane	0.5	
Toluene	0.2	99.5
m-xylene	0.1	
o-xylene	0.1	
Pressure (kPa)	202.6	
Temperature (^{o}C)	30	
Flowrate (kmol/h)	1000	

a) Building up the simulation basic (10 marks)

- Based on information given, list all four variables defined for this case.

  (3 marks)
- What is the phase of this mixture?

  (2 marks)
- Briefly explain how to make this mixture in a vapour phase?

  (3 marks)
- What is the boiling temperature of this mixture? Screenshot the feed information.

  (2 marks)

b) Distillation columns sequence analysis (12 marks)

- Define a direct sequence.

  (3 marks)
- Manually draw the direct sequence for this Feed by showing corresponding component at all product streams.

  (3 marks)
- Define an indirect sequence.

  (3 marks)

- Manually draw the indirect sequence for this Feed by showing corresponding component at all product streams.

(3 marks)

c) Distillation columns sequence simulation analysis (14 marks)

- Simulate the direct sequence in (b) using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this direct sequence.

(2 marks)

- Simulate the indirect sequence in (b) using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this indirect sequence.

(2 marks)

d) Driving force distillation columns sequence analysis (14 marks)

- Develop and plot the driving force curves for this Feed.

(5 marks)

- Synthesize and manually draw this sequence by showing corresponding component at all product streams.

(2 marks)

- Simulate this sequence using Short-Cut distillation column. Screenshot the Aspen HYSYS simulation.

(5 marks)

- Analyse the total energy required for this sequence.

(2 marks)