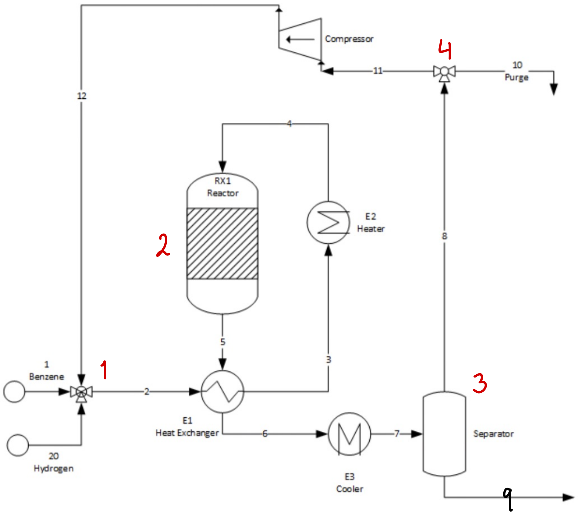
Øving 4

Problem 1

Cyclohexane may be produced by hydrogenation of benzene according to the reaction

$$C_6H_6 + 3\,H_2 = C_6H_{12}$$

The structure of the synthesis part of the process is shown on the flowsheet below:



Stream	Amount	Temperature	Pressure
Benzene (1)	15 m^3/h	100 F	540 psig
Hydrogen (20)	ca 550 kmol/h	100 F	540 psig
Hydrogen recycle (12)	ca 1700 kmol/h	150 F	540 psig

The hydrogen feed, stream 20, contains 2.75 mol% methane.

Unit	Temperature (F)	Pressure loss (psi)
E1, hot side		5
E1, cold side		10
E2, out	300	5
E3, out	120	5
RX1, out	435	15

The heat exchanger E1 has area of 60 m^2, $U = 625$ W/(m^2C). The benzene conversion over the reactor is to be 99.9%.

Design specifications are:

- The maximum allowed concentration of methane (inert) is 10 mol % in the recycle stream, stream 12 or 11.
- Reactor feed, stream 4, should have a molar hydrogen/benzene ratio of 12:1

The possible variables to be adjusted are

- The amount of hydrogen feed; stream 20
- The purge; stream 10
- or the recycle flow, stream 11 and 12

Hints: Using the Spreadsheet, you may import data from the streams in the flowsheet and use these for calculation of certain parameters to control the process, using Adjust.

a) Before you do any simulation in Hysys, estimate approximate values for amounts and composition of the main flows in the flow sheet. Assume perfect split in the separator; only H_2 and methane over top. Vary the divider split ratio and see the effect on recycle composition. You may use hand calculations or a Python (Matlab) script.

b) Plan the simulation by adding the units that you may need in addition to the ones shown on the flow sheet. Where would you put Adjust to obtain the wanted result?

c) Do the simulation in Hysys and submit a printout of the results.

a)

$$F_{C_6H_6,1} = \frac{\rho \cdot \dot{V}}{M} = 167{,}8 \text{ kmol/h}$$

$$T = 311 \text{ K}$$

$$La \; F_i = \begin{bmatrix} F_{C_6H_6,i} \\ F_{H_2,i} \\ F_{C_6H_{12},i} \\ F_{CH_4,i} \end{bmatrix}$$

$$F_{H_2,20} = (1-0{,}0275)\cdot 550 \text{ kmol/h} = 534{,}875 \text{ kmol/h}$$

$$F_{CH_4,20} = 0{,}0275 \cdot 550 \text{ kmol/h} = 15{,}125 \text{ kmol/h}$$

1. Mixer

$$F_2 = F_1 + F_{11} + F_{20}$$

2. Reactor

$$X = [\overset{0{,}999}{\overset{\shortparallel}{X_{C_6H_6}}}, 0, 0, 0]$$

$$\xi = X \cdot F_2$$

$$N = \begin{bmatrix} -1 \\ -3 \\ 1 \\ 0 \end{bmatrix}$$

$$F_5 = (I + NX)F_2$$

3. Separator

$$a_k = [0 \;\; 1 \;\; 0 \;\; 1]$$

$$A = \text{diag}(a_k)$$

$$F_8 = AF_5$$

$$F_{ut} = (I - A)F_5 = F_5 - F_8$$

4. Divider

$$F_{11} = \alpha \cdot F_8$$

$$F_{10} = (1-\alpha)F_8$$

For å løse, må finne $\mathbb{F}_{11}$:

Kombinerer massebalansene:

$$\mathbb{F}_{11} = \alpha \cdot \mathbb{F}_8 = \alpha \cdot \mathbb{A} \mathbb{F}_5 = \alpha \cdot \mathbb{A}(\mathbb{I} + \mathbb{N}\mathbb{X}) \cdot \mathbb{F}_2$$

$$\mathbb{F}_{11} = \alpha \cdot \mathbb{A}(\mathbb{I} + \mathbb{N}\mathbb{X}) \cdot (\mathbb{F}_1 + \mathbb{F}_{11} + \mathbb{F}_{20})$$

$$\Rightarrow \left(\mathbb{I} - \underbrace{\left[\alpha \cdot \mathbb{A}(\mathbb{I} + \mathbb{N}\mathbb{X})\right]}_{=\mathbb{M}}\right) \mathbb{F}_{11} = \alpha \cdot \mathbb{A}(\mathbb{I} + \mathbb{N}\mathbb{X})(\mathbb{F}_1 + \mathbb{F}_{20})$$

$$(\mathbb{I} - \mathbb{M}) \mathbb{F}_{11} = \mathbb{M}(\mathbb{F}_1 + \mathbb{F}_{20})$$

Import python

De molare komponentstrømmene [kmol/h]:

Stream	FC6H6	FH2	FC6H12	FCH4	F_tot
F1	168	0	0	0	168
F20	0	535	0	15	550
F2	168	1140	0	302	1611
F5	0	637	168	302	1107
F8	0	637	0	302	940
F9	0	0	168	0	168
F10	0	32	0	15	47
F11	0	605	0	287	893

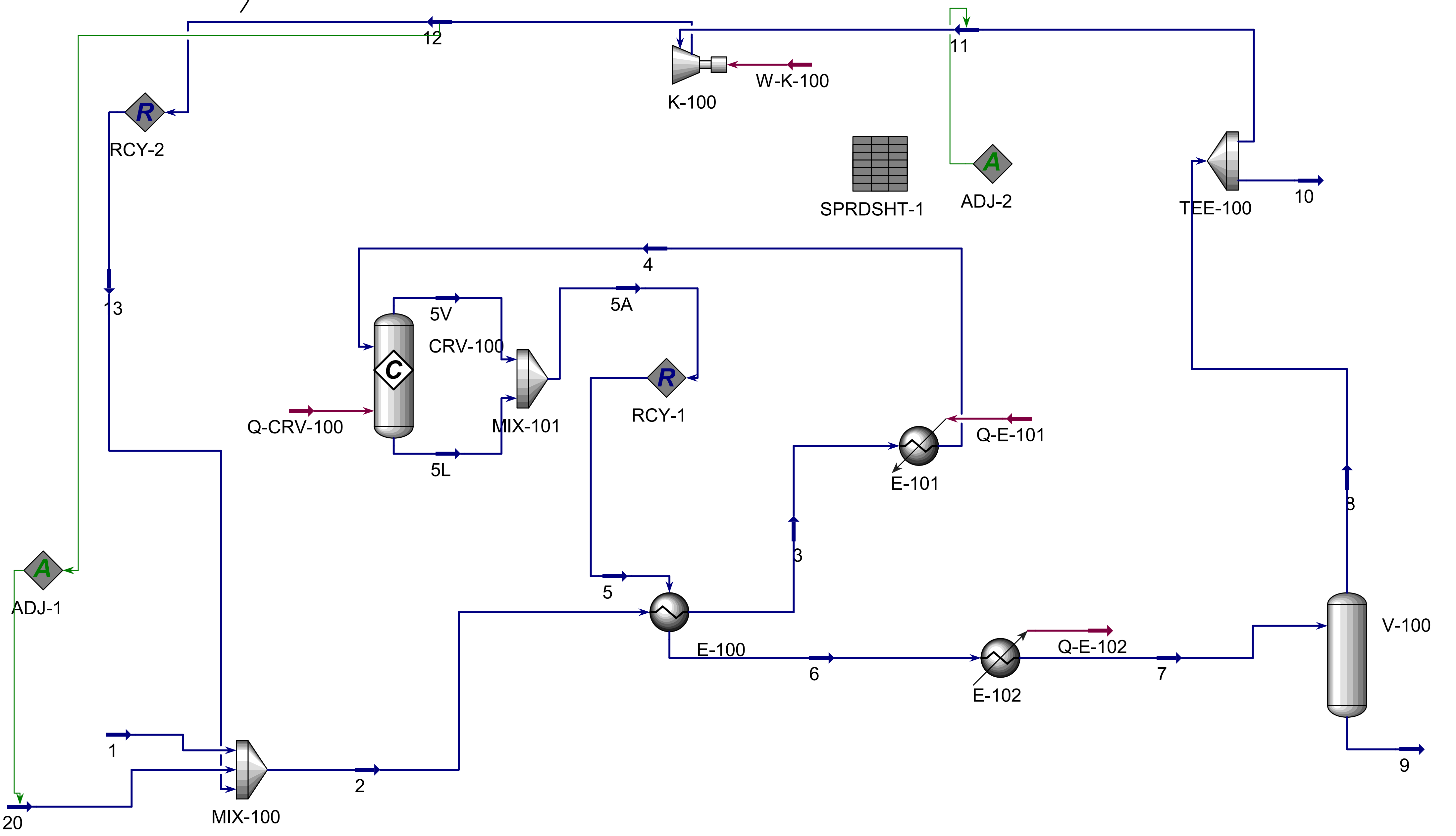
Sammensetning av strømmene:

Stream	XC6H6	XH2	XC6H12	XCH4
F1	1.0	0.0	0.0	0.0
F20	0.0	0.97	0.0	0.03
F2	0.1	0.71	0.0	0.19
F5	0.0	0.58	0.15	0.27
F8	0.0	0.68	0.0	0.32
F9	0.0	0.0	1.0	0.0
F10	0.0	0.68	0.0	0.32
F11	-0.0	0.68	0.0	0.32

For alpha = 0.95, the recycle ratio is 1.24, and X_CH4,11 = 0.32.

Resirkuleringsstrømmen endrer ikke sammensetning når man endrer splittfaktoren.

b)


12
11
K-100
W-K-100
RCY-2
SPRDSHT-1
ADJ-2
TEE-100
10
4
13
5V
5A
CRV-100
RCY-1
Q-CRV-100
MIX-101
Q-E-101
5L
E-101
8
3
ADJ-1
5
E-100
V-100
Q-E-102
6
7
E-102
1
9
2
20
MIX-100

Workbook: Case (Main)

Material Streams

Fluid Pkg: All

Name	1	20	2	3	5
Vapour Fraction	0.0000	1.0000	0.9295	0.9939	1.0000
Temperature (C)	37.78 *	37.78 *	46.82	110.2	223.9 *
Pressure (kPa)	3824 *	3824 *	3824	3756	3618 *
Molar Flow (kgmole/h)	169.4	665.3 *	2387	2387	1879 *
Mass Flow (kg/h)	1.323e+004	1598	2.166e+004	2.166e+004	2.166e+004
Liquid Volume Flow (m3/h)	15.00 *	19.65	84.72	84.72	73.30
Heat Flow (kJ/h)	8.798e+006	-1.129e+006	-4.615e+006	5.352e+006	-2.051e+007
Name	6	4	5V	5L	5A
Vapour Fraction	0.9824	1.0000	1.0000	0.0000	1.0000
Temperature (C)	115.0	148.9 *	223.9 *	223.9	223.9
Pressure (kPa)	3583	3721	3618	3618	3618
Molar Flow (kgmole/h)	1879	2387	1879	0.0000	1879
Mass Flow (kg/h)	2.166e+004	2.166e+004	2.166e+004	0.0000	2.166e+004
Liquid Volume Flow (m3/h)	73.30	84.72	73.30	0.0000	73.30
Heat Flow (kJ/h)	-3.048e+007	9.166e+006	-2.051e+007	-0.0000	-2.051e+007
Name	7	9	8	11	10
Vapour Fraction	0.9085	0.0000	1.0000	1.0000	1.0000
Temperature (C)	48.89 *	48.89	48.89	48.89	48.89
Pressure (kPa)	3549	3549	3549	3549	3549
Molar Flow (kgmole/h)	1879	172.0	1707	1552 *	155.0
Mass Flow (kg/h)	2.166e+004	1.413e+004	7533	6849	683.8
Liquid Volume Flow (m3/h)	73.30	18.20	55.10	50.09	5.002
Heat Flow (kJ/h)	-3.954e+007	-2.547e+007	-1.407e+007	-1.279e+007	-1.277e+006
Name	12	13			
Vapour Fraction	1.0000	1.0000			
Temperature (C)	57.79	57.80 *			
Pressure (kPa)	3824 *	3824 *			
Molar Flow (kgmole/h)	1552	1552 *			
Mass Flow (kg/h)	6849	6833			
Liquid Volume Flow (m3/h)	50.09	50.07			
Heat Flow (kJ/h)	-1.237e+007	-1.228e+007			

Compositions

Fluid Pkg: All

Name	1	20	2	3	5
Comp Mole Frac (Cyclohexane)	0.0000 *	0.0000 *	0.0079	0.0079	0.1002 *
Comp Mole Frac (Hydrogen)	0.0000 *	0.9725 *	0.8493	0.8493	0.8086 *
Comp Mole Frac (Benzene)	1.0000 *	0.0000 *	0.0710	0.0710	0.0001 *
Comp Mole Frac (Methane)	0.0000 *	0.0275 *	0.0717	0.0717	0.0911 *
Name	6	4	5V	5L	5A
Comp Mole Frac (Cyclohexane)	0.1002	0.0079	0.1002	0.1002	0.1002
Comp Mole Frac (Hydrogen)	0.8086	0.8493	0.8086	0.8086	0.8086
Comp Mole Frac (Benzene)	0.0001	0.0710	0.0001	0.0001	0.0001
Comp Mole Frac (Methane)	0.0911	0.0717	0.0911	0.0911	0.0911
Name	7	9	8	11	10
Comp Mole Frac (Cyclohexane)	0.1002	0.9733	0.0122	0.0122	0.0122
Comp Mole Frac (Hydrogen)	0.8086	0.0152	0.8885	0.8885	0.8885
Comp Mole Frac (Benzene)	0.0001	0.0009	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0911	0.0106	0.0992	0.0992	0.0992
Name	12	13			
Comp Mole Frac (Cyclohexane)	0.0122	0.0122 *			
Comp Mole Frac (Hydrogen)	0.8885	0.8893 *			
Comp Mole Frac (Benzene)	0.0000	0.0000 *			
Comp Mole Frac (Methane)	0.0992	0.0985 *			

Energy Streams

Fluid Pkg: All

Name	Q-E-101	Q-CRV-100	Q-E-102	W-K-100	
Heat Flow (kJ/h)	3.814e+006	-2.968e+007	9.056e+006	4.234e+005	

* Specified by user.

Workbook: Case (Main) (continued)

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
MIX-100	Mixer	1 20 13	2	No	500.0 *
MIX-101	Mixer	5V 5L	5A	No	500.0 *
E-100	Heat Exchanger	2 5	3 6	No	500.0 *
E-101	Heater	3 Q-E-101	4	No	500.0 *
CRV-100	Conversion Reactor	4 Q-CRV-100	5L 5V Q-CRV-100	No	500.0 *
RCY-1	Recycle	5A	5	No	400.0 *
RCY-2	Recycle	12	13	No	400.0 *
E-102	Cooler	6	7 Q-E-102	No	500.0 *
V-100	Separator	7	9 8	No	500.0 *
TEE-100	Tee	8	11 10	No	500.0 *
K-100	Compressor	11 W-K-100	12	No	500.0 *
SPRDSHT-1	Spreadsheet			No	500.0 *
ADJ-2	Adjust			No	3500 *
ADJ-1	Adjust			No	3500 *

* Specified by user.