1. HEAT INTEGRATION (GROUP)

1.1 Introduction and Process Description

Maleic anhydride is a cyclic dicarboxylic organic compound with the chemical formula $C_4H_2O_3$. It is the acid anhydride of maleic acid and can be obtained by removing water molecules from its structure. It is also known as 2-5-Furandione, 108-31-6, cis-butenedioic anhydride and toxillic anhydride. Exposure to maleic anhydride can cause eye and respiratory irritation and chronic bronchitis. Therefore, it is important to handle it with proper care.

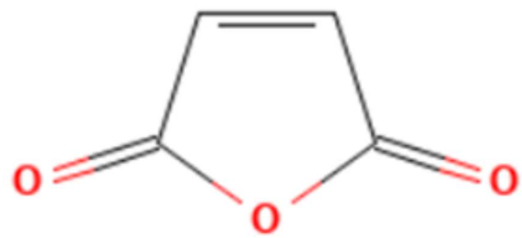


Figure 1.1.1: Structural formula of maleic anhydride

Maleic anhydride is a colorless or white crystalline solid with a pungent odor at room temperature. It can also be a liquid or gas. It has a boiling point of 202 ℃ and a melting point of 52.85 ℃ It has a bifunctional reactivity of its double bond and is used in various industrial applications such as the production of unsaturated polyester resins, coatings, agriculture products, lubricants and fuel oil. It is obtained via the thermal dehydration of maleic acid from an aqueous solution or by azeotropic distillation.

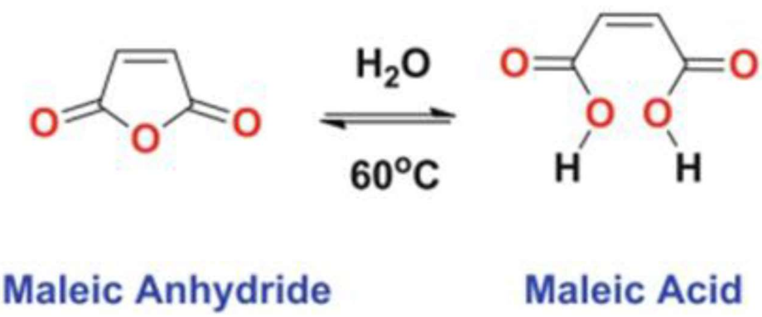


Figure 1.1.2: Reactions from maleic anhydride to maleic acid

Optimization problem can be solved manually. However, computer-aided solutions are more widely used as it can reduce time solving and more efficient in solving complicated problems. Simulation software such as MATLAB, Excel solver, GAMS, Aspen HYSYS and Aspen Energy are usually used to solve optimization problems and they are chosen based on the characteristics of the problem.

Process Description

The main reaction in the production of maleic anhydride from n-butane is an exothermic partial oxidation reaction which carried out in multitubular fixed bed reactors using a catalyst containing vanadium oxide and phosphorus oxide. The synthesis of maleic anhydride using partial oxidation of a linear hydrocarbon was expressed as the equation below:

$$C_4H_y + \left(1 + \frac{y}{4}\right) O_2 \rightarrow C_4H_2O_3 + (\frac{y}{2} - 1)H_2O$$

Where the hydrogen in hydrocarbon y is equivalent to 10 of hydrogen in n-butane and 8 in n-butene. The process generates maleic anhydride, with carbon dioxide, carbon monoxide and water as by-products. To obtain the main product, dibutyl phthalate is used as an organic solvent in the absorbers. The customer requires the production of approximately 36,800 m^3/year of 98% pure maleic anhydride by partially oxidizing n-butane and oxygen on a VPO catalyst, which is oxidized using a stream od pure oxygen and nitrogen.

Main reaction in the reactor:

$$C_4H_{10} + 3.5O_2 \rightarrow C_4H_2O_3 + 4H_2O$$
$$C_4H_{10} + 5.5O_2 \rightarrow 2CO + 2CO_2 + 5H_2O$$

The process involves several stages, starting with heating of pure n-butane in Heater E-101 to produce fresh n-butane. Next, fresh n-butane is then mixed in M-101 with the resulting mixture from Mixer MIX-104, which contain nitrogen and a recycle stream from main system which includes oxygen from TEE-102 recycled via RCY-2 and compressed by K-101 before heated in E-106 then directed into Mixer M-104. Th resultant mixture from M-101 mixed with the resultant mixture from M-102 and fed into conversion reactor CRV-100.

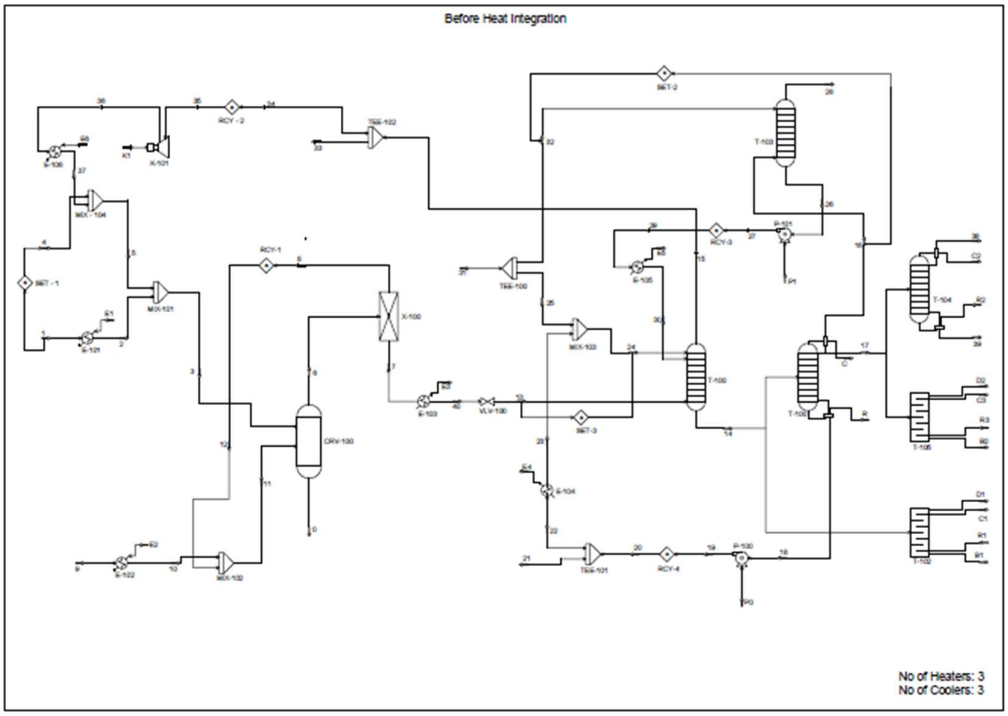
After leaving CRV-100, The mixture is sent to Component Splitter X-100 which separates oxygen from the reactor. The oxygen is then recycled RCY-1 back to CRV-100 via M-102, while the remaining gaseous products, unreacted n-butane and nitrogen are separated from bottom of the splitter and sent to E-103 for cooling. The pure oxygen is heated in E-102 and mixed with the recycled oxygen from RCY-1 before being sent back to CRV-100.

In TEE-100, the fresh organic solvent line (dibutyl phthalate) is split into 2 streams, one of which is mixed with the cooled E-104 recycle RCY-4 stream in Mixer MIX-103 and sent to the main absorber T-100, while the other stream is used as an inlet for scrubber T-103 and consists of pure organic solvent. The overhead gaseous stream from T-103 is vented, while the bottom stream is recycled RCY-3 back into T-100 after being cooled with E-105.

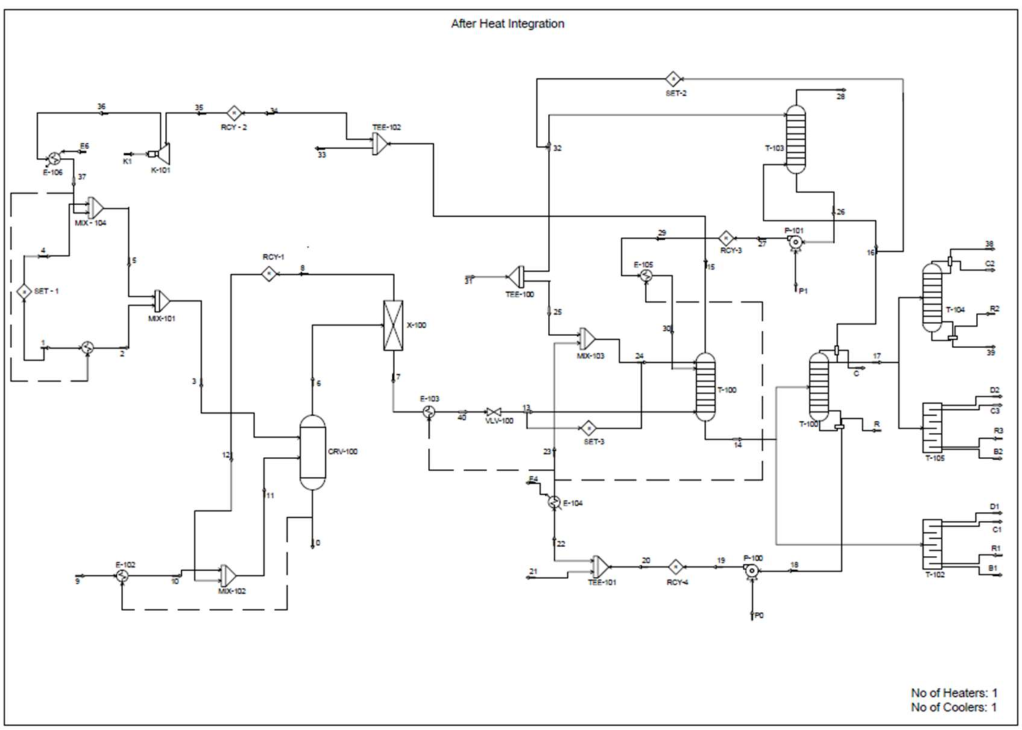
In TEE-101, the recycle RCY-4 from condenser of the distillation column T-101 is split into 2 streams. One stream is cooled with E-104 and sent to Mixer MIX-103, while the other stream is purged. T-100 has 3 inlet streams: the mixture of fresh solvent line with the recycle RCY-4 stream, the cooled gaseous products from E-103 and the recycle RCY-3 stream from the bottom outlet of T-103, which contains dibutyl phthalate organic solvent, water, maleic anhydride and unreacted n-butane. The overhead stream of T-100 is the main recycle RCY-2 stream, consisting mainly of nitrogen and n-butane with smaller percentage of other oxidation products. The stream leaving T-100 through the bottom of the column is made up of organic solvent and absorbed maleic anhydride. This stream becomes the inlet liquid feed for T-101 and shortcut column T-102, with distillate consisting of maleic anhydride, water and dibutyl phthalate exiting from the bottom of the column.

Finally in distillation column T-101, the gaseous product recycled as RCY-4 leaving from the condenser, while the liquid line exiting from the reboiler, consisting mainly of maleic anhydride and water. This liquid stream is then sent to distillation column T-104 and shortcut column T-105. For the T-104, the excess water is recovered via the overhead while the maleic anhydride leaving from the bottom of T-104 as main product. For T-105, the distillate is mainly the water and maleic anhydride exiting from the bottom of T-105 as main product.

1.2 Process Flow Diagram (Before Integration)



1.3 Process Flow Diagram (After Integration)



1.4 Stream Data for Heat Integration

Throughout the simulation, there have been temperature restrictions concerning liquid mixtures of water and maleic anhydride to prevent reactions that lead to maleic acid and fumaric acid. The gaseous mixture and organic solvent interaction are considered ideal mixtures. The process data for the production of Maleic Anhydride was obtained through pipeline tracing and interviews with experienced operators. Based on the Block Flow Diagram, there are a few streams that require a heating and cooling process. In order to reach high reaction temperatures and pressures, a large amount of steam is supplied to the sterilization process. Steam is obtained from the heating of water to reach high temperature and pressure, then a vaporizer is needed to change the water from the liquid phase into the vapor phase.

The steam supplied is not suitable to be utilized in the heat integration as there is a phase change from the liquid state to the vapor state. After the sterilization process, the steam energy excess with two possible areas such as discharging as condensate (H1) and discharging to the atmosphere as exhaust steam (H2). The steam condensate (H1) from the sterilization process is unable to be recovered due to the presence of overheating because the sterilization process involves high temperatures, which can cause the steam condensate to be too hot to handle or reuse without further treatment. On the other hand, it could be caused by contamination. It is possible for the steam condensate from the sterilization procedure to include bacteria or other microbes, making it unfit for reuse. However, it is necessary to cool down the steam condensate (H1) before discharging. H1 exits from the sterilization process at 374.5***°C*** and undergoes a cooling process in a cooler to decrease its temperature to 55***°C***. Since the temperature is within the sensible heat region, the steam condensate does not undergo a phase change process during the cooling process. The exhaust steam (H2) exits at 240***°C*** from the sterilization process and undergoes a cooling process in a cooler to reduce its temperature to 30***°C*** without phase change. The exhaust steam still contains a high amount of heat energy and can undergo a heat exchange process with a cold stream instead of wasting its heat energy in the cooler.

The next process is the threshing process and the output from the threshing process which is(C1) requires increasing its temperature before entering the digestion process. The (C1) increases its temperature from 200 ***°C*** to 370 ***°C*** in a heater without phase change. Besides, there is a stream of steam supplied into the digestion process. The steam can be obtained by heating the water in a vaporizer with a phase change. After that, a stream of hot water (C2) enters a screw press. Water at atmospheric conditions requires increasing its temperature from 229***°C*** to 370***°C*** to reduce the viscosity from the screw press.

In the final stage of the production, there will be Maleic Anhydride (H3) produced. The (H3) collected at the temperature of 148.6***°C*** and it is required to be cooled down to 60***°C*** nefore sending it to the storage tank. Besides, the sludge from the bottom of setting tank enters the decanter to remove solid waste such as mud or sand before entering a separator to recover possible oil contained in the sludge. The separator also has a hot water (C3) input to enhance its separation efficiency. Therefore, water (C3) is required to increase its temperature from 86.89 ***°C*** to 370***°C*** in a heater.

The supply temperature, and target temperature of six hot and cold streams in Maleic Anhydride production process are summarized in Table 1.4.1 below. Furthermore, the mole flow (kmol/hour) and heat capacity (J/kmol.K) are also tabulated in Table 1.4.2 and 1.4.3.

Table 1.4.1: Summary of six hot and cold streams.

Stream	**Hot/Cold Stream No.**	**Equipment Stream**	**Tsupply (°C)**	**Ttarget (°C)**	**FCp (kJ/s.K)**	**Tsupply, shifted**	**Ttarget, shifted**
Hot	H1	E-103	374.50	55.00	291.30	369.50	50.00
Hot	H2	E-104	240.00	30.00	30.09	235.00	25.00
Hot	H3	E-105	148.60	60.00	5.59	143.60	55.00
Cold	C1	E-101	200.00	370.00	4.47	205.00	375.00
Cold	C2	E-102	229.00	370.00	5.94	234.00	375.00

Cold	C3	E-106	86.89	370.00	255.70	91.89	375.00

Table 1.4.2: Mass Flow rate of each stream.

Mole Flow (kmol/hour)	**C1**	**C2**	**C3**	**H1**	**H2**	**H3**
H_2O	0.00	0.00	1835.36	2192.19	0.00	12.30
Maleic Anhydride	0.00	0.00	0.00	73.75	0.00	7.23
Dibutyl Phthalate	0.00	0.00	0.00	0.00	227.10	37.72
Nitrogen	0.00	0.00	27437.73	30670.73	0.00	0.00
Oxygen	0.00	670.00	0.00	0.00	0.00	0.00
CO_2	0.00	0.00	198.75	224.50	0.00	0.00
CO	0.00	0.00	198.83	224.58	0.00	0.00
n-Butane	100.00	0.00	186.13	200.15	0.00	0.00

Table 1.4.3: Heat Capacity of each stream.

Heat Capacity (J/kmol.K)	**C1**	**C2**	**C3**	**H1**	**H2**	**H3**
H_2O	35863	36025	35325	35638	77078	75462
Maleic Anhydride	128540	128540	128540	128540	163760	163760
Dibutyl Phthalate	-	-	-	-	477000	477000
Nitrogen	29868	29948	29623	29761	-	-
Oxygen	31770	31916	31265	31563	-	-
CO_2	46186	46532	44952	45689	-	-
CO	30154	30252	29845	30022	-	-
n-Butane	160871	163726	150784	156788	-	-

1.5 Manual Calculation

Pinch Analysis is conducted using two different approaches, namely the composite curve and the Problem Table Algorithm. The analysis involves converting temperatures into shifted temperatures. The formula below is used to calculate the shifted temperatures for both the hot and cold streams.

$$T_{hot,shi} = T_{hot} - \frac{\Delta T_{min}}{2}$$

$$T_{cold,shifted} = T_{cold} + \frac{\Delta T_{min}}{2}$$

The minimum temperature difference (ΔTmin) is a crucial factor that drives the heat exchange between the hot and cold streams, and its value varies for each process. A higher value of ΔTmin indicates a lower capital cost for the heat exchanger. Selecting the appropriate ΔTmin is essential for minimizing the total cost of the heat exchanger. In the chemical industrial sector, ΔTmin of 10 °C is typically chosen, which is suitable for this type of process. Table 1.5.1 presents the necessary data for conducting the pinch analysis.

Table 1.5.1: Data Required for Pinch Analysis

Stream	Hot/Cold Stream No.	Equipment Tag No.	T_{supply} (°C)	T_{target} (°C)	FCp (kJ/s·K)	$T_{supply,shifted}$	$T_{target,shifted}$
Hot	H1	E-103	374.5	55	291.3	369.5	50
	H2	E-104	240	30	30.09	235	25
	H3	E-105	148.6	60	5.585	143.6	55
Cold	C1	E-101	200	370	4.469	205	375
	C2	E-102	229	370	5.940	234	375
	C3	E-106	86.89	370	255.7	91.89	375

1.5.1 Composite Curve

The composite curve is a graphical tool used to display hot streams, cold streams, and the potential for heat transfer between them. This method is used to identify the heat cascade in a process. To construct the composite curve, the shifted temperatures obtained from the process streams are plotted against their respective enthalpies. This results in the creation of one curve for the hot streams and another curve for the cold streams. Prior to constructing the composite curve, the hot and cold stream lines need to be established. The data analyzed in Table 1.5.1 is used to construct these stream lines, with Figure 1.5.1 illustrating the hot stream line and Figure 1.5.2 showing the cold stream line. The enthalpy change (ΔH) is plotted on the temperature axis, and a sample calculation for determining the enthalpy change is provided below.

Sample calculation for enthalpy change, ΔH for hot stream line interval 50$°C$ to 25$°C$:

$$\Delta H = \sum FC_p \times \Delta T$$

$$\Delta H = \sum FC_p \times \Delta T$$

$$\Delta H = (291.3 + 30.09) \times (55 - 50)$$

$$\Delta H = 1607\ kJ/s$$

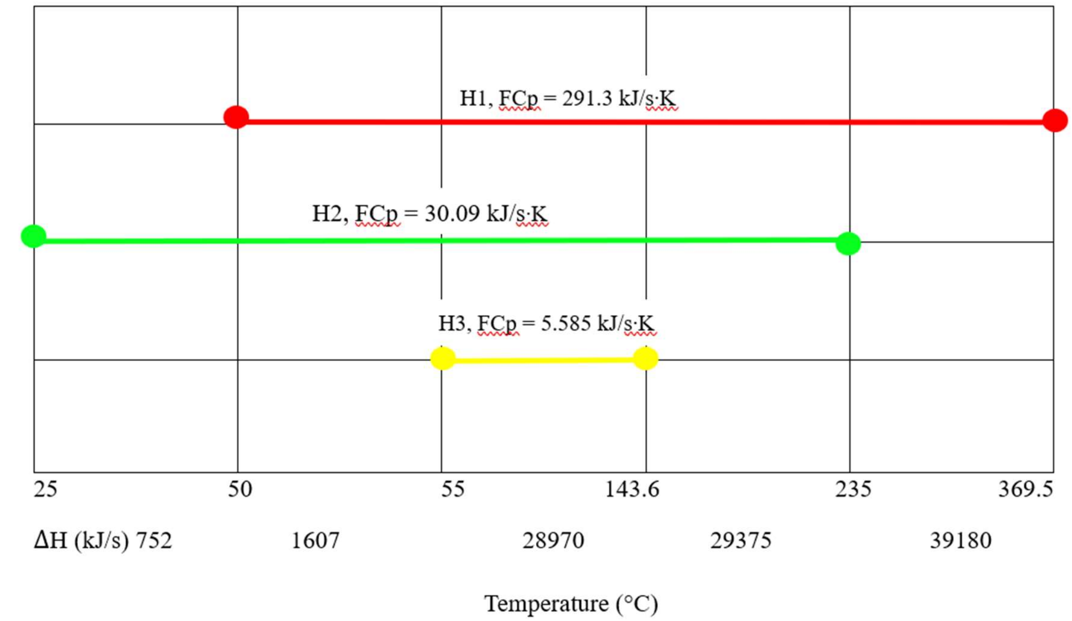


Figure 1.5.1: Hot Stream Line

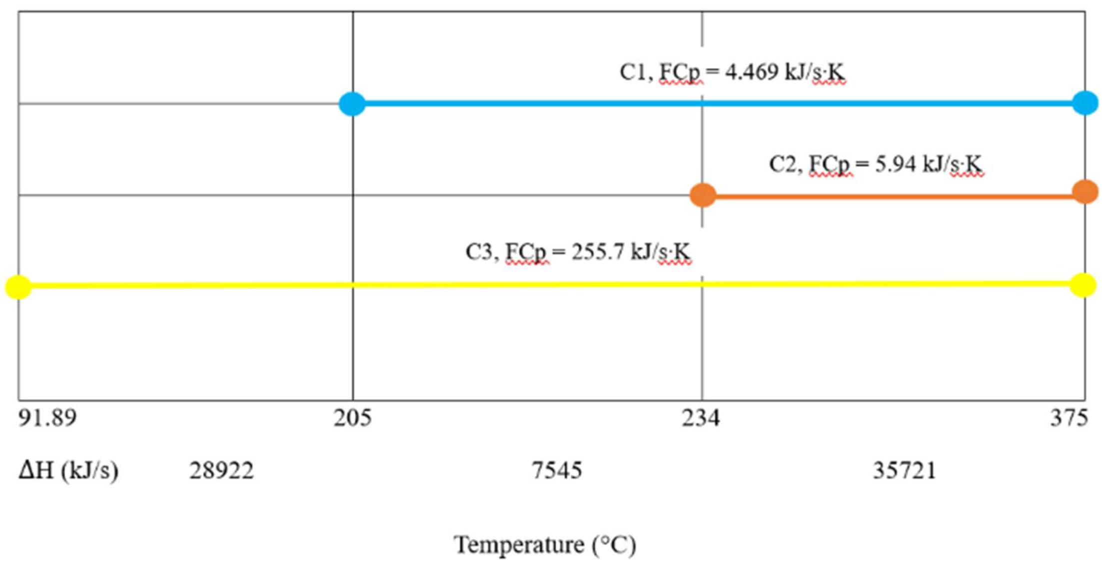


Figure 1.5.2: Cold Stream Line

Table 1.5.2: Data of Stream Line for Construction of Composite Curve

Stream	$T_{shifted}(°C)$	$\Delta H\ (kJ/s)$	$\Delta H\ (MJ/s)$	$Cumulative\ \Delta H\ (MJ/s)$
Hot	25	-	-	0
	50	752	0.752	0.752
	55	1607	1.607	2.359
	143.6	28970	28.97	31.329
	235	29375	29.375	60.704
	369.5	39180	39.18	99.884
Cold	91.89	-	-	0
	205	28922	28.922	28.922
	234	7545	7.545	36.467
	375	35721	35.721	72.188

Following the establishment of the hot and cold stream lines, the shifted temperature composite curve is then constructed using the data presented in Table 1.5.2. Figure 1.5.3 displays the resulting shifted temperature composite curve.

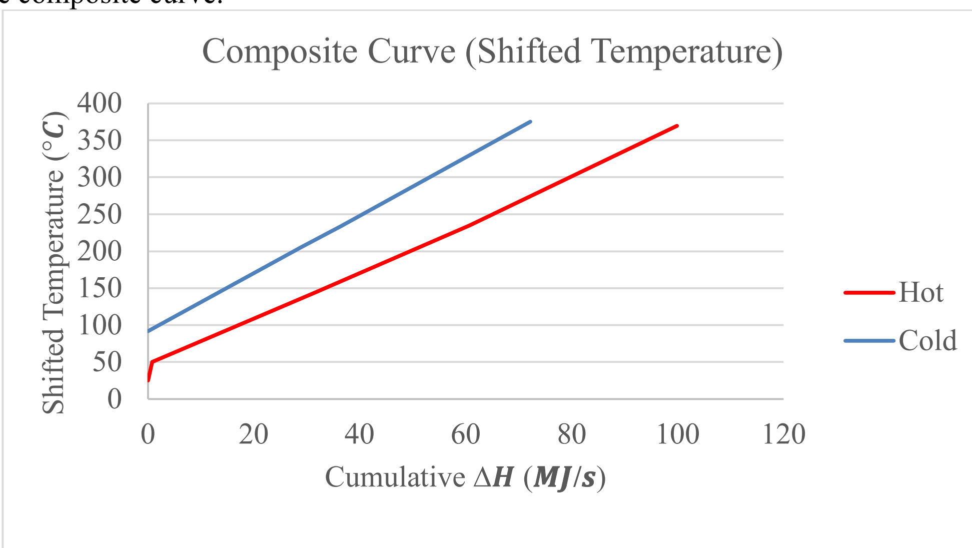


Figure 1.5.3: Composite Curve of Shifted Temperature against Cumulative ΔH

When constructing composite curves, it is important to position them relative to each other in a way that ensures the hot composite curve (representing the cooling process) is always above the cold composite curve (representing the heating process). Next, the cold stream is shifted to the right side of the graph until it aligns with the end of the hot stream on the x-axis. This results in the creation of the shifted cold stream composite curve, as illustrated in Figure 1.5.4.

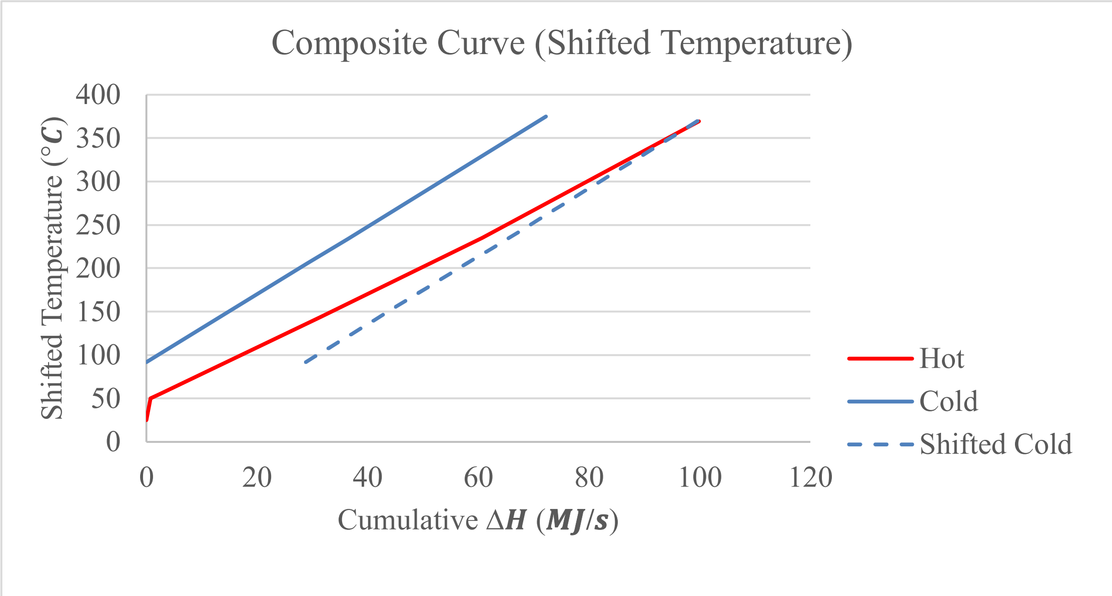


Figure 1.5.4: Shifted Cold Stream in Shifted Temperature Composite Curve

The analysis of Figure 1.5.4 indicates that this is a threshold problem. This is because the cold stream line is completely overlapped by the hot stream line, which indicates that the cooling stream can be fully satisfied by the heating stream. In threshold problems, a pinch point violation occurs, as the pinch point does not exist in this type of scenario. As a result, there is neither a hot pinch temperature nor a cold pinch temperature in this case. The shifted temperature composite curve is then used to determine the minimum cooling utility, which represents the enthalpy difference between the starting point of the hot curve and the shifted cold curve. This minimum cooling utility can be identified by referring to Figure 1.5.5.

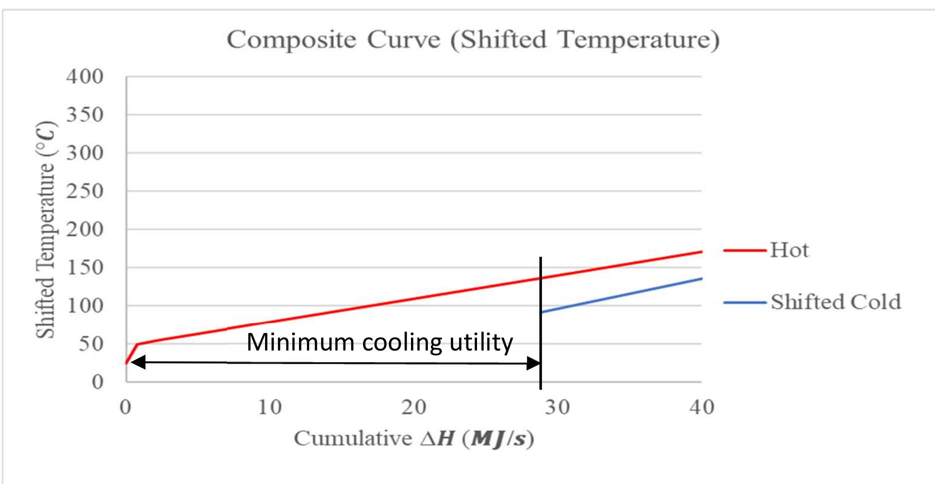


Figure 1.5.5: Minimum Cooling Utility Obtained from the Actual Composite Curve

From figure 1.5.5, the minimum cooling utility is 28.822 MJ/s. In short, composite curve results shows minimum cooling utility is 28822 kJ/s while the minimum heating utility is 0 kJ/s.

1.5.2 Problem Table Algorithm (PTA)

The Problem Table Algorithm is an alternative numerical method for identifying the pinch point, minimum heating and cooling utilities, which differs from the graphical approach of the composite curve.

In this case, the data presented in Table 1.5.1 is used to carry out the algorithm. The enthalpy change (ΔH) for each temperature range is calculated using the following equation. The resulting calculations and PTA analysis are presented in Table 1.5.3.

$$\Delta H = \sum FC_{p,hot} - \sum FC_{p,cold} \times \Delta T$$

Sample calculation for ΔH:
By taking a shifted temperature range of $235°C$ to $369.5°C$:

$$\Delta H = (\sum FC_{p,hot} - \sum FC_{p,cold}) \times \Delta T$$
$$\Delta H = (H1 - C1 - C2 - C3) \times (369.5 - 235)$$
$$\Delta H = (291.3 - 4.469 - 5.94 - 255.7) \times (369.5 - 235)$$
$$\Delta H = 3388.1895\ kJ/s$$

Table 1.5.3: Problem Table Algorithm Stream Analysis

$T_{shifted}$ (°C)	ΔT (°C)	Streams						$FC_{p,hot} - FC_{p,cold}$	ΔH (kJ/s)
			H1	H2	H3	C1	C2	C3		
		FC_p ($kJ/s \cdot K$)	291.3	30.09	5.585	4.469	5.94	255.7		
375										
	5.5								266.109	1463.5995
369.5										
	134.5								25.191	3388.1895
235										
	1								55.281	55.281
234										
	29								61.221	1775.409
205										
	61.4								65.69	4033.366
143.6										
	51.71								71.275	3685.6303
91.89										
	36.89								326.975	12062.108
55										
	5								321.39	1606.95
50										
	25								30.09	752.25
25										

After the calculation of ΔH, two heat cascades, namely infeasible heat cascade and feasible heat cascade were conducted. Firstly, infeasible heat cascade was constructed. In order to find the minimum utility, the biggest negative value of cumulative delta H need to be found out to build another cascade table. However, the infeasible heat cascade does not contain negative value of cumulative delta H in this case, thus it is impossible to proceed to build the feasible heat cascade. Therefore, it has been established that the case being analyzed is a threshold problem. The infeasible heat cascade table is constructed and presented in Table 1.5.4.

Table 1.5.4: Infeasible Heat Cascade

$T_{shifted}(°C)$	$\Delta H\ (kJ/s)$	Cummulative $\Delta H\ (kJ/s)$
	0.000	
375		0.0000
	1463.5995	
369.5		1463.5995
	3388.1895	
235		4851.7890
	55.281	
234		4907.0700
	1775.409	
205		6682.4790
	4033.366	
143.6		10715.8450
	3685.63025	
91.89		14401.4753
	12062.1078	
55		26463.5830
	1606.95	
50		28070.5330
	752.25	
25		28822.7830

The location of the pinch point and the minimum heating utility can be determined from the value of zero at the top of the cumulative delta H column in Table 1.5.4. Additionally, the minimum cooling utility can be obtained from the last value of the cumulative delta H column. In this particular case, the minimum cooling utility is determined to be 28822.783 kJ/s, which is almost identical to the value obtained from the composite curve method.

Table 1.5.5: Comparison of Results from Composite Curve and Problem Table Algorithm

	Composite Curve	Problem Table Algorithm
Minimum Heating Utility (kJ/s)	0	0
Minimum Cooling Utility (kJ/s)	28822	28822.783

1.6 Construction of Heat Exchanger Network Diagram

Above Pinch Region

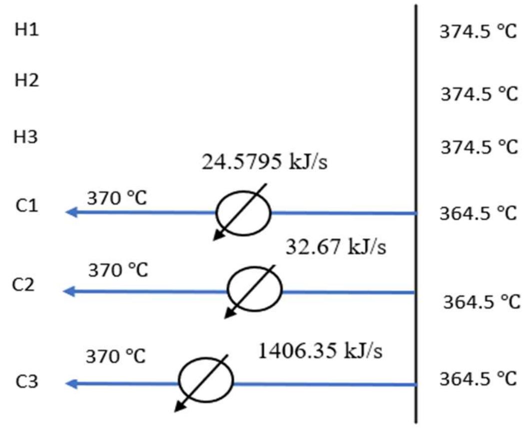


Figure 1.6.1 Above Pinch Region

Table 1.6.1: Stream and Relative Data involved in Above Pinch Region

Stream	FCp (kJ/ s.K)	Heat Load, ΔH (kJ/s)
C1	4.469	24.5795
C2	5.940	32.67
C3	255.7	1406.35

<u>Calculation of Head Load, ΔH (kJ/h)</u>

$\Delta H\ (C1) \quad = FCp \times \Delta T$

$\quad = 4.469 \times (370 - 364.5)$

$\quad = 24.5795$ kJ/s

$\Delta H\ (C2) \quad = FCp \times \Delta T$

$\quad = 5.940 \times (370 - 364.5)$

$\quad = 32.67$ kJ/s

$\Delta H\ (C3) \quad = FCp \times \Delta T$

$\quad = 255.7 \times (370 - 364.5)$

$\quad = 1406.35$ kJ/s

$$\text{Total heat } load\ or\ total \text{ heating utilities} = 24.5795\,\frac{\text{kJ}}{\text{s}} + 32.67\,\frac{\text{kJ}}{\text{s}} + 24.5795\,\frac{\text{kJ}}{\text{s}}$$

$$= 1463.5995\,\frac{\text{kJ}}{\text{s}}$$

$$= 5.269 \times 10^6\,\frac{\text{kJ}}{\text{h}}$$

Figure 1.6.1 above shows the above pinch region diagram of the heat exchanger network diagram. At this region, it is to recover the maximum heat recovery from the streams above by using the pinch technology and pinch point obtained above. In above pinch region, it only contains 3 stream which are C1, C2 and C3 stream. Since there are no hot streams to provide the heat exchange, heaters are required. C1 stream require a heater which provide 24.5795 kJ/s of heat load, C2 stream require a heater which provide 32.67 kJ/s of heat load while C3 stream require a heater with 1406.35 kJ/s of heat load. Therefore, there are total of 3 heaters with total of heating utilities of 5.269 x $10^6\,\frac{\text{kJ}}{\text{h}}$ in above pinch region.

<u>Below Pinch Region</u>

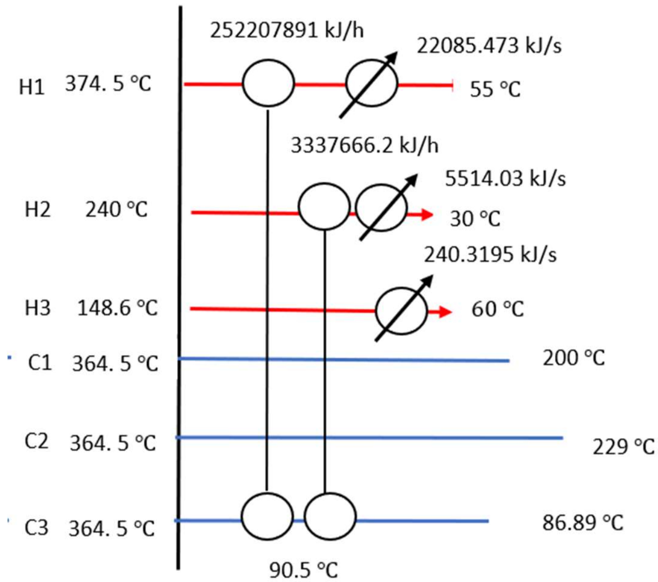


Figure: 1.6.2 Below Pinch Region

Table 1.6.2 Stream and Relative Data involved in Below Pinch Region

Stream	FCp (kJ/ s.K)	Heat Load, ΔH (kJ/s)
H1	291.3	-93070.35
H2	30.09	-6318.90
H3	5.585	-494.831
C1	4.469	735.1505
C2	5.940	804.87
C3	255.7	70984.877

Calculation of Head Load, ΔH (kJ/h)

ΔH (H1) $= FCp \times \Delta T$
$= 291.3 \times (55 - 374.5)$
= -93070.35 kJ/s

ΔH (H2) $= FCp \times \Delta T$
$= 30.09 \times (30 - 240)$
= -6318.90 kJ/s

ΔH (H3) $= FCp \times \Delta T$
$= 5.585 \times (60 - 148.6)$
= -494.831 kJ/s

ΔH (C1) $= FCp \times \Delta T$
$= 4.469 \times (364.5 - 200)$
= 735.1505 kJ/s

ΔH (C2) $= FCp \times \Delta T$
$= 5.940 \times (364.5 - 229)$
= 804.87 kJ/s

ΔH (C3) $= FCp \times \Delta T$
$= 255.7 \times (364.5 - 86.89)$
= 70984.877 kJ/s

Total heat $load\ or\ total$ cooling utilities = -93070.35 kJ/s + -6318.90 kJ/s + -494.831 kJ/s +
=735.1505 kJ/s + 804.87 kJ/s + 70984.877 kJ/s
$= 27359.1835\ \frac{\mathrm{kJ}}{\mathrm{s}}$
$= 9.8493 \times 10^{7}\ \frac{\mathrm{kJ}}{\mathrm{h}}$

The above pinch region, there is a total of 6 streams involved. All the streams are involved in and thus there are several heat integration solutions to be performed as the optimal solutions. The design considerations of the below pinch are opposed to the above pinch design. According to the objective mentioned in the below pinch design, cooling utilities are only allowed to be installed in below pinch region to remove the heat energy to reach the target temperature in hot stream. The selection between H2 and C3 is chosen. Although the Fcp of stream H2 is smaller than Fcp of C3, heat integration can be performed as the temperature different between hit the minimum temperature approach of 10 ℃. The selection between H1 and C3 is chosen. The Fcp of stream H1 is larger than C3. So, it can be chosen because it meets the criteria at below pinch region.

Heat Exchange Network Design

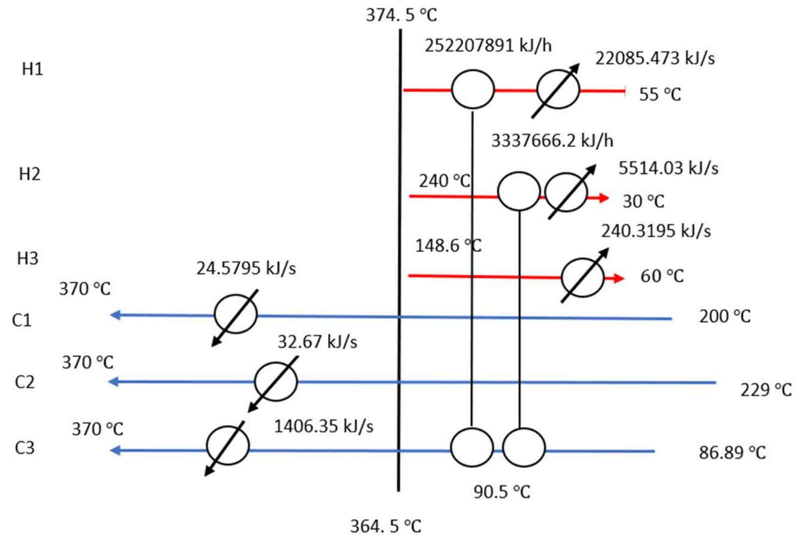


Figure 1.6.3: Overall Heat Exchange Network Diagram

The overall heat exchange network diagram is shown as Figure 1.6.3. The above pinch region diagram is combined with below pinch diagram to generate the overall heat exchange network diagram. There are total of 8 heat exchangers involved with 2 heat exchangers between process to process, 3 heating utilities from stream C1, C2 and C3 and 3 cooling utilities at stream H1, H2 and H3. The total heat utility involved is 5.269 x $10^6 \frac{\text{kJ}}{\text{h}}$ while total cold utility is 9.8493 x $10^7 \frac{\text{kJ}}{\text{h}}$.

1.7 Aspen Energy Analyzer

Name		Inlet T [C]	Outlet T [C]	MCp [kJ/C-h]	Enthalpy [kJ/h]	Segm.	HTC [kJ/h-m2-C]	Flowrate [kg/h]	Effective Cp [kJ/kg-C]	DT Cont. [C]
H1		374.5	55.0	1.049e+006	3.351e+008		720.0	---	---	Global
H2		240.0	30.0	1.083e+005	2.275e+007		720.0	---	---	Global
H3		148.6	60.0	2.011e+004	1.781e+006		720.0	---	---	Global
C1		200.0	370.0	1.609e+004	2.735e+006		720.0	---	---	Global
C2		229.0	370.0	2.138e+004	3.015e+006		720.0	---	---	Global
C3		86.9	370.0	9.205e+005	2.606e+008		720.0	---	---	Global
New										

Figure 1.7.1: Input Data of All Streams into Aspen Energy Analyzer

There are a total of 3 hot streams and 3 cold streams from the production of the maleic anhydride process. The heat exchanger network diagram is verified via the simulation in Aspen Energy Analyzer. Data such as the name of stream, inlet, outlet temperature, and Mcp value are typed into Aspen Energy Analyzer. The other information is set as default and simulated by Aspen Energy Analyzer.

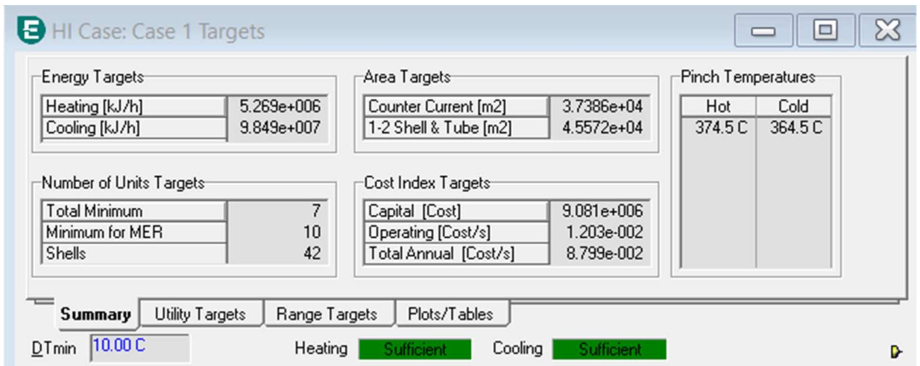


Figure 1.7.2: Check for Targets

Under the selecting open target view option, the hot pinch temperature, cold pinch temperature, minimum cooling, and heating utility can be obtained at this table. The minimum temperature, ΔTmin is 10 °C. The minimum heating utility and cooling utility is 5.269 x $10^6 \frac{kJ}{h}$ and 9.849 x $10^7 \frac{kJ}{h}$ respectively. The hot pinch temperature and cold pinch temperature is 374.5 °C and 364.5 °C respectively. The pinch temperature is 369.5 °C.

Name		Inlet T [C]	Outlet T [C]	Cost Index [Cost/kJ]	Segm.	HTC [kJ/h-m2-C]	Target Load [kJ/h]	Effective Cp [kJ/kg-C]	Target Flowrate [kg/h]	DT Cont. [C]
Fired Heat (1000)		1000.0	400.0	4.249e-006		399.6	5.269e+006	1.000	8782	Global
Cooling Water		20.0	25.0	2.125e-007		1.350e+00	9.849e+007	4.183	4.709e+006	Global
<empty>										

Process Streams | Utility Streams | Economics | Options | Notes

Set Up Operations | Convert to HI Project | Hot Sufficient | Cold Sufficient

Figure 1.7.3: Selection of Utilities

When the exchange of heat between the process stream had reached maximum, heating, and cooling utilities were needed so that the process can be satisfied. According to Figure 1.7.3, the heating utility such as fired heat is selected because its temperature is higher than 370 °C. This heating utility is to provide heat to 3 of the cold streams which are C1, C2, and C3. While the cooling utility selected is cooling water to cool the hot stream which is H1, H2, and H3. Below figure 1.7.3, the status is changed from red color to green color indicating that the utilities selected were sufficient.

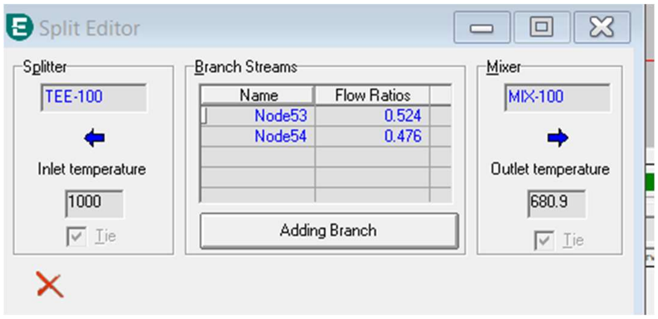


Figure 1.7.4: Splitter added into Cold Utility Stream

A splitter is added into the cold utility stream which is cooling water stream. The flow ratios is entered as 0.524 and 0.476.

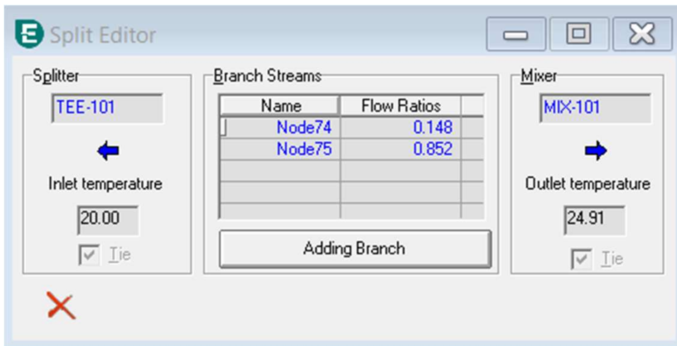


Figure 1.7.5: Splitter added into Hot Utility Stream

A splitter is added into hot utility stream with flow ratios of 0.148 and 0.852.

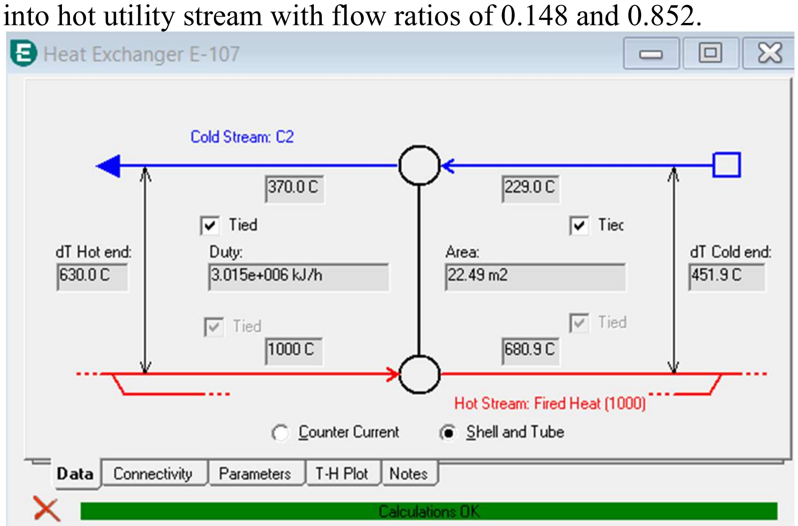


Figure 1.7.6: Heating Utility installed in Stream C2

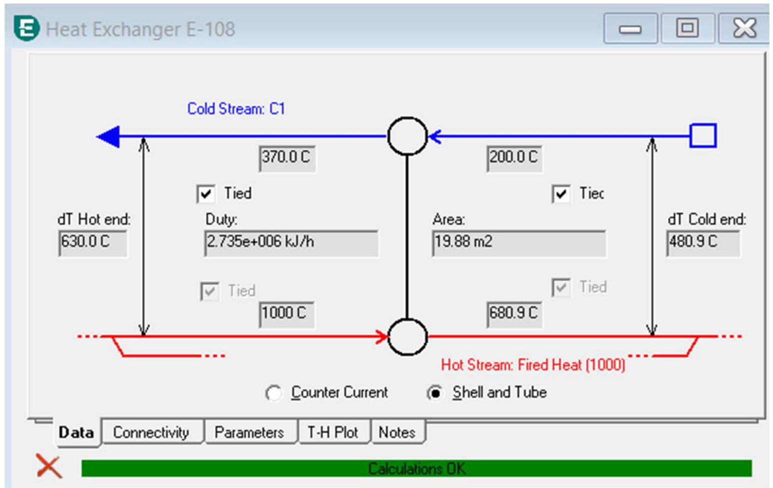


Figure 1.7.7 Heating Utility Installed in Stream C1

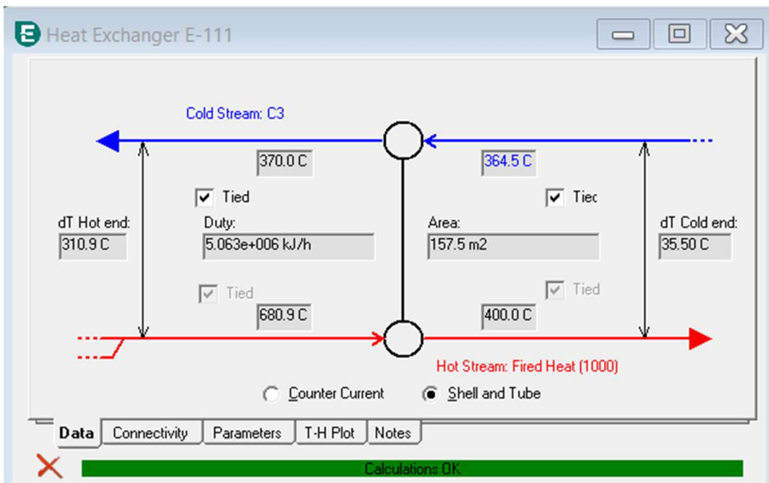


Figure 1.7.8: Heating Utility installed in Stream C3

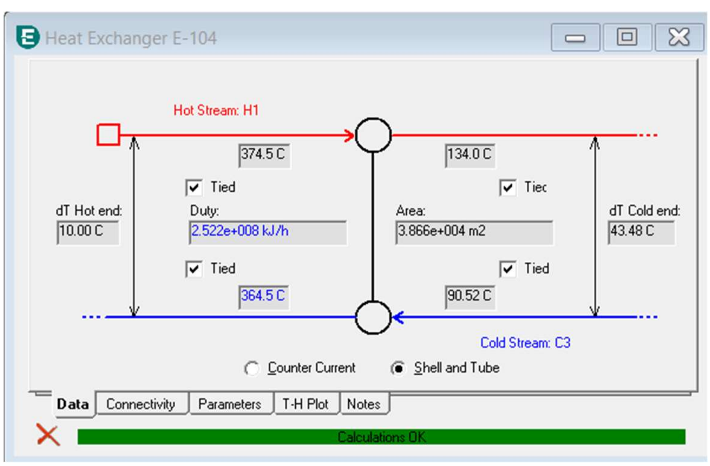


Figure 1.7.9: Heat Exchange between H1 and C3

Based on Figure 1.7.9 above, the heat exchanger is added for heat exchange between stream H1 and stream C3. The outlet temperature of C3 is set as 364.5 ℃ and inlet temperature is set as 90.52℃ The tied is tick. At the inlet temperature of hot stream is 374.5 ℃ and the outlet temperature is 134 ℃. The tied is tick. The heat duty required by the heat exchanger is 2.522 x $10^8 \frac{kJ}{h}$.

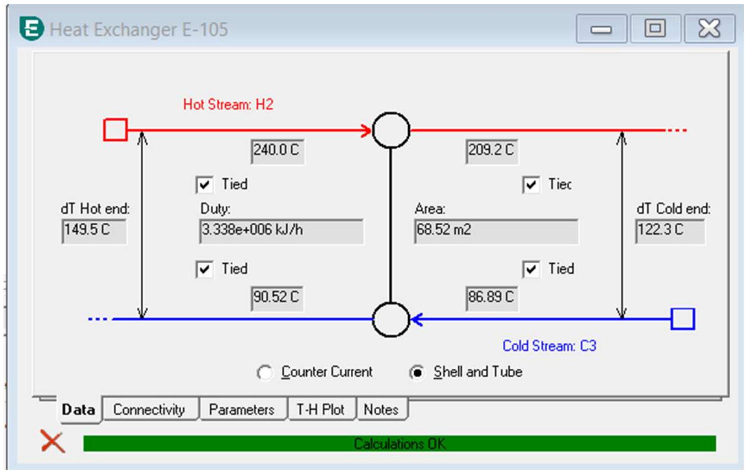


Figure 1.7.10: Heat Exchange between H2 and C3

Based on Figure 1.7.10 above, the heat exchanger is added for heat exchange between stream H2 and stream C3. The outlet temperature of C3 is set as 90.52 °C and inlet temperature is set as 86.89 °C The tied is tick. The inlet temperature of a hot stream is 240 °C and the outlet temperature is 209.2 °C. The tied is tick. The heat duty required by the heat exchanger is $3.338 \times 10^6 \frac{kJ}{h}$.

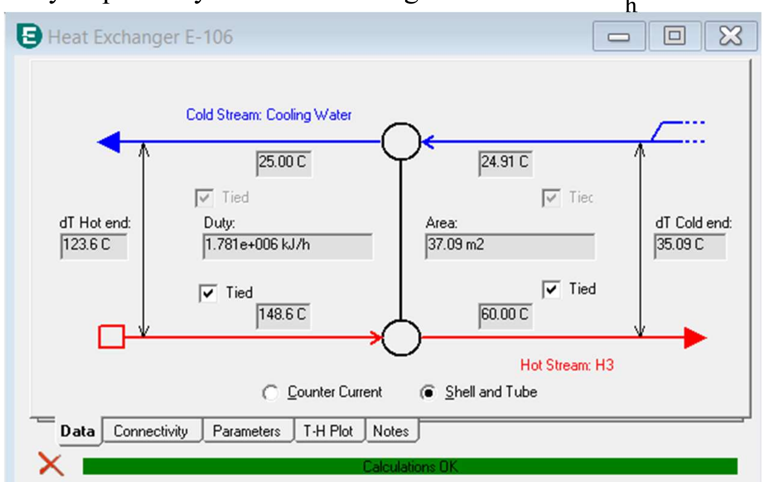


Figure 1.7.11 Cooling Utility installed into Stream H3

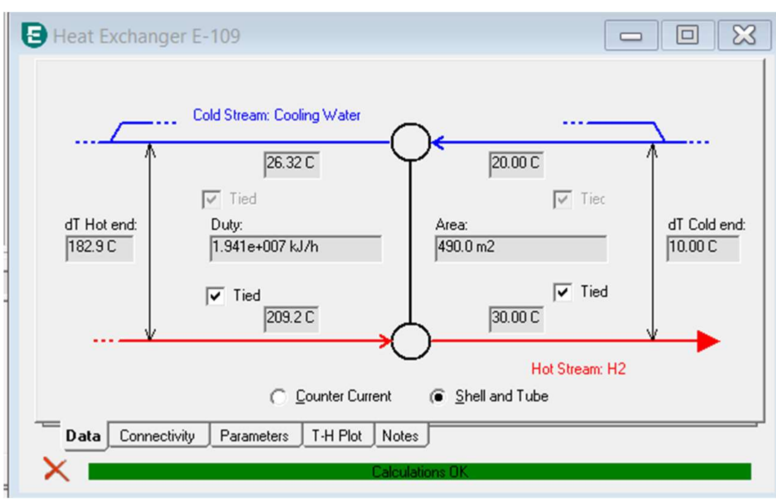


Figure 1.7.12 Cooling Utility installed into Stream H2

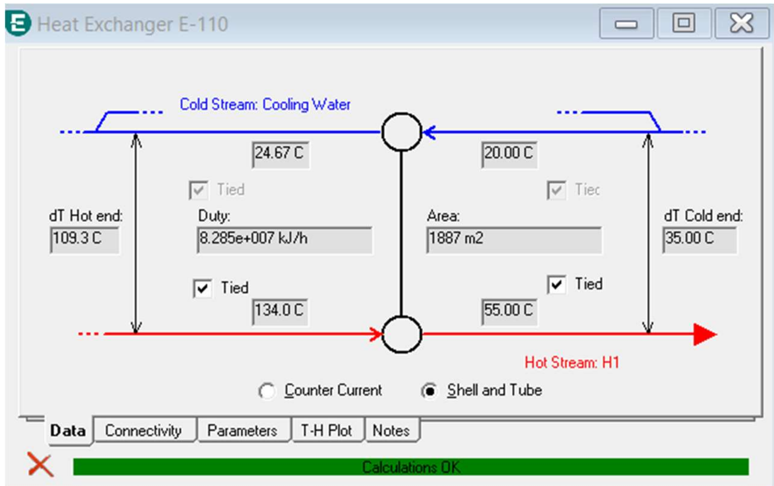


Figure 1.7.13 Cooling Utility installed into Stream H1

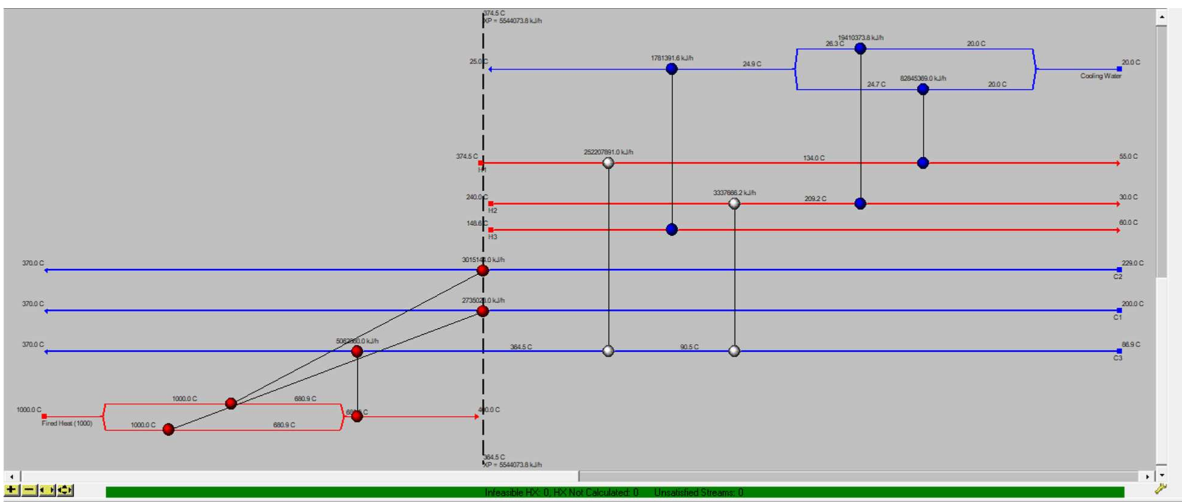


Figure 1.7.14: Heat Exchange Design Diagram

Figure 1.7.14 shows the heat exchange design diagram that is constructed by using Aspen Energy Analyzer. All the lines do not appear dotted means that all the streams had successfully satisfied. In conclusion, the minimum heating duty in streams C1, C2, and C3 are 3015144 kJ/h, 2735028 kJ/h , and 5062860 kJ/h respectively. The total heating duty is 1.081 x $10^7 \frac{kJ}{h}$. The minimum cooling utility in stream H1, H2 and H3 are 252207891$\frac{kJ}{h}$, 1781391.6 $\frac{kJ}{h}$ and 3337666.2 $\frac{kJ}{h}$ respectively. The total cooling duty is 1.04 x $10^8 \frac{kJ}{h}$. The difference in total heating and cooling utility generated in Aspen Energy Analyzer and manual calculation is due to the reason simplifying assumptions. Aspen Energy Analyzer will make several assumptions when performing the calculations. Another reason is convergence issues. Aspen Energy Analyzer will iterate various combinations of heat exchangers when it solves problems until it reaches a convergence point. Furthermore, Aspen Energy Analyzer may use more complex algorithms and models to optimize the heat exchanger network which will lead to different results.

2. INDIVIDUAL PART

2.1 Optimizing maleic anhydride microcapsules size for use in self-healing epoxy-based coatings for corrosion protection of aluminum alloy (Jee Pei Qi 1805656)

Introduction and Description of the Problem

Since self-healing coatings have become so important recently, there has been a growing demand to optimize process variables for efficient control of the functions of the coatings for long-lasting application. The usage of central composite design (CCD) of the response surface methodology (RSM) is still one of the most efficient and dependable methods for getting desired optimized attributes. Therefore, the goal of this work was to create a suitable model for optimizing microcapsule size for usage in the production of microcapsules based on maleic anhydride for self-healing function in faulty epoxy coating.

Microsoft Excel tool, known as "Solver," was employed in this study to help attain this goal. The program is frequently utilized for optimization modeling. In order to guard against corrosion, it may choose the ideal microcapsule size needed for Maleic Anhydride synthesis. In addition, to guarantee the accuracy and dependability of the optimization model, the production variables in this case study stirring speed, and time are taken into account

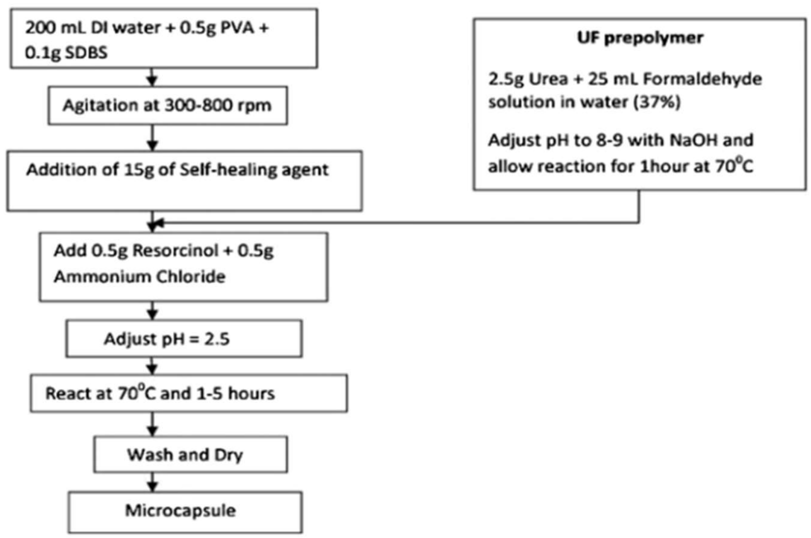


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Figure 2.1.1: Flow diagram of optimizing maleic anhydride microcapsule size

Problem Statement and formulation of Objective Function

The synthesis of the maleic anhydride microcapsule uses the capsule-based self-healing technique since it has a less complicated manufacturing procedure and a lower production cost. The shape of the microcapsules is significantly influenced by the stirring rate and duration. To obtain a long shelf life during storage and good adherence to the polymer matrix, the process variables (such as stirring speed and duration) must be optimized. The goal of the present research is to provide a suitable model for microcapsule size optimization to be employed in the production of maleic anhydride-based microcapsules for self-healing function in faulty epoxy coating systems. Hence, minimization is used to obtain optimized microcapsule size. According to Xin Wang (2021), smaller microcapsules often enable better coating dispersion and more effective self-healing. However, a microcapsule size between 1 and 10 microns is often advised for aluminum alloys. This is due to the possibility that bigger microcapsules might hinder the coating's ability to adhere to the substrate, whilst smaller microcapsules could not have enough healing potential.

Decision Variables:
X1= Stirring rate (rpm)
X2= Duration (hours)

Objective Function: Minimize the microcapsule size appropriate for aluminum alloy coating, y

$$y = 12.08 + 4.6_{x1} + 5.8_{x2} - 1.43_{x1x2} + 3.5^2_{x1} + 8.89^2_{x2}$$

<u>Presentation and Description of Data to be Used</u>

Standard order	**Stirring speed (X1) (rpm)**	**Time (X2) (hours)**	**Experimental particle size (μm)**
1	**300**	**2**	**12.92**
2	**800**	**2**	**26.48**
3	**300**	**4**	**24.6**
4	**800**	**4**	**32.44**
5	**196.45**	**3**	**14**
6	**903.55**	**3**	**24.89**
7	**550**	**1.59**	**20.06**
8	**550**	**4.41**	**40.4**
9	**550**	**3**	**12.08**

Table 2.1.1: Tabulation of data from case study

Objective Function:

$$y = 12.08 + 4.6_{x1} + 5.8_{x2} - 1.43_{x1x2} + 3.5^2_{x1} + 8.89^2_{x2}$$

Subjected to constraints:

300X1 + 2X2 >=12.92 ----------(Standard order 1)
800 X1 + 2X2 >= 26.48 ---------(Standard order 2)
300 X1 + 4X2 >=24.6 -----------(Standard order 3)
800X1 + 4X2 >=32.44 ----------(Standard order 4)
196.45X1 + 3X2 >=14 ----------(Standard order 5)
903.55X1 + 3X2 >=24.89------- (Standard order 6)
550X1 + 1.59X2 >=20.0 --------(Standard order 7)
550X1 + 4.41X2 >=40.4 --------(Standard order 8)
550X1 + 3X3 >=12.08 ----------(Standard order 9)

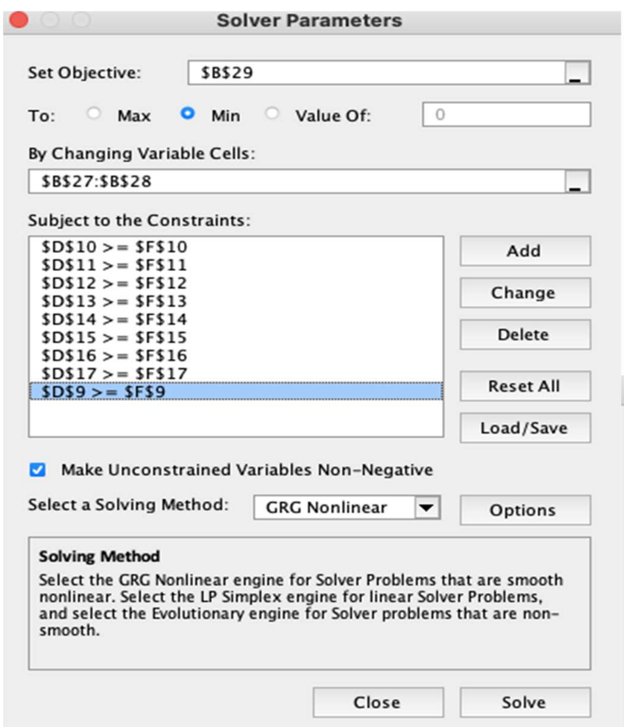
<u>Solution from Microsoft Excel</u>

Figure 2.1. shows that a Microsoft Excel spreadsheet is deployed for mathematical modeling followed by optimization using Solver. At first, the objective function is to optimize the microcapsule size, and the decision variables are entered into the cells. Next, the constraints are being constructed as well. Under cells X1 and X2, any number can be assigned because Solver will adjust the optimum values after undergoing an optimization procedure, and in this case, 1 is assigned to both cells. The data is extracted from the case study, and the formula is entered following the original formula found in the case study while X1 and X2 are equal to 1 as assigned earlier and 33.44 is calculated.

Objective Function						
Optimise microcapsule size	$y = 12.08 + 4.6x_1 + 5.8x_2 - 1.43_{x1x2} + 3.5^2_{x1} + 8.89^2_{x2}$					
Decision Variable						
X1	Stirring Speed (rpm)					
X2	Time (hrs)					
Standard Order	Stirring speed	Time		Symbol	Experimental particle size	
1	300	2	302	>=	12.92	
2	800	2	802	>=	26.48	
3	300	4	304	>=	24.6	
4	800	4	804	>=	32.44	
5	196.45	3	199.45	>=	14	
6	903.55	3	906.55	>=	24.89	
7	550	1.59	551.59	>=	20.06	
8	550	4.41	554.41	>=	40.4	
9	550	3	553	>=	12.08	
Optimise microcapsule size						
Stirring speed X1	1					
Time X2	1					
Optimised microcapsule size	33.44					

Figure 2.1.2: Before optimization (Excel Spreadsheet)

Moreover, under the data tab, Solver can be utilized to solve this minimization problem. Figure 2.1.3, shows that the objective function, changing variables, and constraints are selected. Before pressing "Solve", it is to ensure that the 'Min' is ticked and solving method of "GRC Nonlinear" is chosen. Figure 2.1.4 indicates that the Solver has successfully found a solution that satisfied all the constraints and optimal conditions. Next, under the Reports section, click on 'Answer', 'Sensitivity and 'Limits' to get the reports for overall views of the optimum values as shown in Figures s1.6, 2.1.7, and 2.1.8.



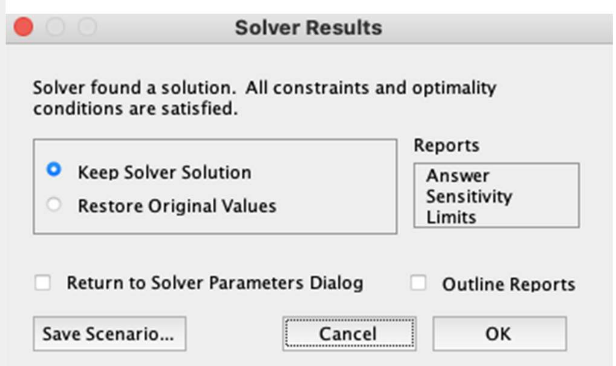


Figure 2.1.3: Solver Parameter **Figure 2.1.4: Solver Results**

Figure 2.1.5 shows that the Solver has optimized X1 and X2 values to 0.082 rpm and 0 hours respectively. Consequently, the microcapsule size has also been optimized to 12.481 μm from 33.44μm. Studies show that epoxy-based self-healing coatings can employ microcapsules with particle sizes between 1 and 12 microns. Because it enables the incorporation of a high concentration of microcapsules into the coating while still maintaining good dispersion and flow properties, this range is frequently preferred. The size and shape of the aluminum alloy substrate that has to be covered must also be taken into account. For instance, bigger microcapsules can be necessary if the substrate has a rough surface in order to achieve enough coverage and adherence. On the other hand, smaller microcapsules could work better if the substrate has a smooth surface.

Objective Function					
Optimise microcapsule size	$y = 12.08 + 4.6x_1 + 5.8x_2 - 1.43_{x1x2} + 3.5^2_{x1} + 8.89^2_{x2}$				
Decision Variable					
X1	Stirring Speed (rpm)				
X2	Time (hrs)				
Standard Order	Stirring speed	Time		Symbol	Experimental particle size
1	300	2	24.6	>=	12.92
2	800	2	65.6	>=	26.48
3	300	4	24.6	>=	24.6
4	800	4	65.6	>=	32.44
5	196.45	3	16.1089	>=	14
6	903.55	3	74.0911	>=	24.89
7	550	1.59	45.1	>=	20.06
8	550	4.41	45.1	>=	40.4
9	550	3	45.1	>=	12.08
Optimise microcapsule size					
Stirring speed X1	0.082				
Time X2	0				
Optimised microcapsule size	12.480734				

Figure 2.1.5: After optimization (Excel Spreadsheet)

Objective Cell (Min)

Cell	Name	Original Value	Final Value
$B$29	Optimised microcapsule size Stirring speed	33.44	12.480734

Variable Cells

Cell	Name	Original Value	Final Value	Integer
$B$27	Stirring speed X1 Stirring speed	1	0.082	Contin
$B$28	Time X2 Stirring speed	1	0	Contin

Constraints

Cell	Name	Cell Value	Formula	Status	Slack
$D$10		65.6	$D$10>=$F$10	Not Binding	39.12
$D$11		24.6	$D$11>=$F$11	Binding	0
$D$12		65.6	$D$12>=$F$12	Not Binding	33.16
$D$13		16.1089	$D$13>=$F$13	Not Binding	2.1089
$D$14		74.0911	$D$14>=$F$14	Not Binding	49.2011
$D$15		45.1	$D$15>=$F$15	Not Binding	25.04
$D$16		45.1	$D$16>=$F$16	Not Binding	4.7
$D$17		45.1	$D$17>=$F$17	Not Binding	33.02
$D$9		24.6	$D$9>=$F$9	Not Binding	11.68

Figure 2.1.6: Answer Report

Variable Cells

Cell	Name	Final Value	Reduced Gradient
$B$27	Stirring speed X1 Stirring speed	0.082	0
$B$28	Time X2 Stirring speed	0	5.613762357

Constraints

Cell	Name	Final Value	Lagrange Multiplier
$D$10		65.6	0
$D$11		24.6	0.01724668
$D$12		65.6	0
$D$13		16.1089	0
$D$14		74.0911	0
$D$15		45.1	0
$D$16		45.1	0
$D$17		45.1	0
$D$9		24.6	0

Figure 2.1.7: Sensitivity Report

Cell	Objective Name	Value
$B$29	Optimised microcapsule size Stirring speed	12.480734

Cell	Variable Name	Value	Lower Limit	Objective Result	Upper Limit	Objective Result
$B$27	Stirring speed X1 Stirring speed	0.082	0	85	250	18835
$B$28	Time X2 Stirring speed	0	0	110	398.5	20035

Figure 2.1.8: Limits Report

There are a few factors that can affect the microcapsule particle size and the frequency and force of particle impacts, the stirring speed can have an impact on the particle size distribution. The likelihood of particle collision rises with stirring speed, which results in a reduction in particle size. The particles might, however, fragment or agglomerate if the stirring speed is too high, increasing the particle size. Secondly, the particle size distribution can also be impacted by the duration of stirring. Due to the constant collisions between the particles, longer stirring times can result in a reduction in particle size. However, if the stirring period is too long, the particles may deteriorate or clump together, increasing the particle size. Last but not least, the connection between stirring speed and time can also be influenced by the starting particle size. To obtain a desirable particle size distribution, for instance, smaller particles can need a lower stirring speed and a shorter stirring time, whereas bigger particles would need a higher churning speed and a longer stirring time.

<u>Justification of selection</u>

The reason why Excel is preferred for this case study is because it is frequently used for general-purpose data analysis and manipulation because it provides a nice user interface. Additionally, it has an integrated optimization tool called Solver that can be used to address a variety of optimization issues. Solver may be used with a range of different optimization techniques and is quite simple to use. Excel is also generally accessible and reasonably priced as compared to other optimization software programs. Problems involving linear and nonlinear programming can be resolved using the robust optimization method integrated into Excel's built-in Solver feature. It is simple to use and may be modified to meet the exact specifications of the issue. Besides, Microsoft Excel Spreadsheet is great for data manipulation. The ability to manipulate data in Excel makes it simple to get data ready for optimization. Users can use built-in functions and formulae to alter data that has been imported from a variety of sources. Charting and visualization of data can be user-friendly when it is being done in Excel Spreadsheets. Users may see the outcomes of the optimization model visually because of Excel's charting and graphing features. Users may be better able to comprehend the issue and explain it to others as a result.

2.2 Optimization Case of Cost of raw Materials in Production of Maleic Anhydride (Abbas,S. 2015) (Choong Yi Jie, 1803104)

Introduction and Description of the Problem

The production of Maleic Anhydride requires the use of raw materials such as n-butane, Dibutyl phthalate solvent (DBP) and Vanadium phosphorus oxide (VPO) as a catalyst. The cost of these raw materials will significantly impact the overall production cost of Maleic Anhydride. Hence, the main objective of this study is to determine the optimum utilization of raw materials that fulfills the production requirements while minimizing the cost of raw materials. It is crucial to note that using more raw materials that exceed the necessary can increase the production cost due to the additional raw material costs.

To achieve this objective, software such as Microsoft Excel "Solver" and GAMS were used in this study. These software packages are commonly used for optimization modelling. It can determine the optimal combination of raw materials required for Maleic Anhydride production in the most cost-effective way. The production requirements, cost of each of the raw materials and any other constraints are taken into consideration to ensure the optimization model is accurate and reliable.

Problem statement and formulation of objective function

According to Kowalsky's (2017), the optimization problem to produce Maleic Anhydride involves an objective function that is subject to several constraints. In this study, the objective function represents the total cost of the raw materials that required for the Maleic Anhydride production which is affected by the amounts of the raw materials used. In a year, the production maleic Anhydride required a minimum of 24281 kg of n-butane, 500,000 kg of dibutyl phthalate solvent (DBP) and 45,000 kg of vanadium phosphorus oxide (VPO) catalyst. The goal of the optimization is to minimize as low as possible the cost of raw materials while fulfilling the production requirements to improve the overall profitability of the production process. The decision variables are first identified, followed by the objective function.

Decision variables:

y_1 = the amount of n-butane required per year

y_2 = the amount of dibutyl phthalate solvent (DBP) required per year

y_3 = the amount of vanadium phosphorus oxide catalyst (VPO) required per year

Objective function: Minimize the total cost of raw materials required, Z

$$Z = 3.92\, y_1 + 247.8\, y_2 + 16.76\, y_3$$

Presentation and Description of Data to be Used

As mentioned previously, the production of maleic anhydride requires some raw materials including n-butane, dibutyl phthalate solvent (DBP) as well as vanadium phosphorus oxide catalyst (VPO). The amount of each of raw material required and the costs are obtained from literature provided by Abbas (2015). The amount required per year, cost per unit as well as the total cost estimated for each of the raw material are tabulated in Table 2.2.1.

Table 2.2.1: Raw Material Cost (Abbas, 2015)

Raw Materials	Amount Required / Year (kg/year)	Cost / Unit (RM / kg)	Total Cost Estimated (RM)
n-butane	24,821	3.92	98,000
Dibutyl phthalate solvent (DBP)	500,000	247.8	124,000,000
Vanadium phosphorus oxide catalyst (VPO)	45,000	16.76	750,000
		Total cost:	**RM 125,000,000 / year**

The objective function and constraints are listed as shown below.

Objective function:

$$\text{Minimize } Z = 3.92\ y_1 + 247.8\ y_2 + 16.76\ y_3$$

Subjected to constraints:

$y_1 \leq 24281$ (n-butane required per year)
$y_2 \leq 500000$ (Dibutyl phthalate solvent (DBP) required per year)
$y_3 \leq 45000$ (Vanadium phosphorus oxide catalyst (VPO) required per year)
$y_1, y_2, y_3 \geq 0$

<u>Solution from Microsoft Excel</u>

The solver function in Microsoft Excel has been utilized to carry out the mathematical modelling and followed by the optimization. Figure 2.2.1 shows the print-screen of the Microsoft Excel Spreadsheet with the assigned value to each decision variable. In the spreadsheet, the objective function and its subjected constraints are shown.

Variables	y1	y2	y3				
	1	1	1	Decision Variables			
Constraints	**y1**	**y2**	**y3**	**Total**		**Limit**	
	1	0	0	1	≤	24821	
	0	1	0	1	≤	500000	
	0	0	1	1	≤	45000	Constraints
	1	0	0	1	≥	0	
	0	1	0	1	≥	0	
	0	0	1	1	≥	0	
Objective Function	**y1**	**y2**	**y3**	**TOTAL COST**			
	3.92	247.8	16.76	268.48		Objective Function	

Figure 2.2.1: Spreadsheet of Microsoft Excel

By using the Excel spreadsheet, all the variables and constraints are tabulated. The red highlighted part shown in Figure 2.2.1 are the values assigned to each decision variables at the beginning to allow the Solver to proceed with the iterations without the starting value of 0 which will fail the iteration. Next, the orange highlighted part shown in Figure 2.2.1 are the functions of all the constraints while the green highlighted part is the desired value of the objective function. The Solver Function is selected to start the optimization of the problem once all the values of each variable and constraints are tabulated properly in the Excel spreadsheet. Figure 2.2.2 shows the Solver Parameters window.

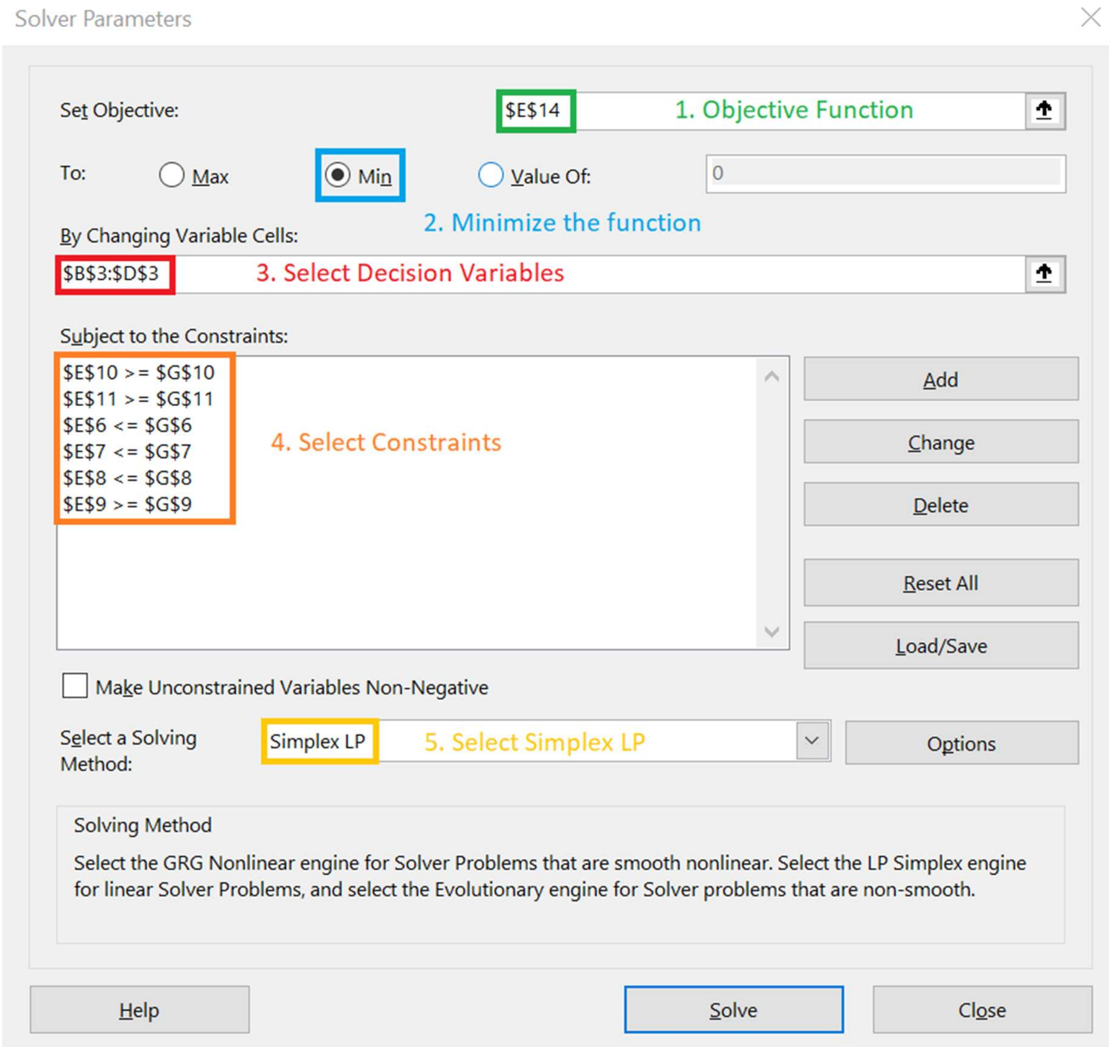


Figure 2.2.2: The Solver Parameters window.

From the Figure 2.2.2, the green highlighted part shows the input of the value of the objective function, which was readily to be minimized, hence the Min button is chosen which is highlighted in blue. The red highlighted part in the Figure 2.2.2 are the decision variables that are readily to be optimized while the orange highlighted part shows the constraints that should be non-negative variables. Once all the constraints involved are computed, the simple Linear Programming (LP) is selected which shown in yellow highlighted part. Then, the solver can run and proceed to optimization. Figure 2.2.3 below shows the optimized value for each of decision variables with the minimized objective function.

Variables	y1	y2	y3	
	24821	500000	45000	Optimized Values

Constraints	y1	y2	y3	Total		Limit
	1	0	0	24821	$\leq$	24821
	0	1	0	500000	$\leq$	500000
	0	0	1	45000	$\leq$	45000
	1	0	0	24821	$\geq$	0
	0	1	0	500000	$\geq$	0
	0	0	1	45000	$\geq$	0

Objective Function	y1	y2	y3	TOTAL COST	
	3.92	247.8	16.76	124751498.3	Optimized Objective Function

Figure 2.2.3: Optimized Values shown by Solver

From Figure 2.2.3, the solver finally identifies a solution that fulfilled all the constraints and at the same time achieve the goal of optimization. The minimized total cost of raw materials of RM124,751,498.30 was obtained and shown in the green highlighted part in Figure 2.2.3, while the red highlighted part shown in Figure 2.2.3 is the minimized amount of each raw material that required in year for the production process. The details of the optimized solution are tabulated in Table 2.2.2. By substituting each of the values given by the Solver into the objective function, the optimized cost of same value as the Solver can be obtained manually.

Table 2.2.2: Details of the Optimized Solution Resulting from Microsoft Excel Solver.

Variables	**y_1(kg/year)**	**y_2 (kg/year)**	**y_3 (kg/year)**
Solver's Solution	24821	500000	45000

Objective function:

$$
\begin{aligned}
\text{Minimize Z} &= 3.92y_1 + 247.8y_2 + 16.76\, y_3 \\
&= 3.92\,(24821) + 247.8\,(500000) + 16.76\,(45000) \\
&= \text{RM}124{,}751{,}498.30
\end{aligned}
$$

<u>Solution from GAMS</u>

To utilize the General Algebraic Modelling System (GAMS) to carry out the mathematical modelling and optimization, The algebraic equations are required to be listed out first. Before generating of the equation, the algebraic variables involved are identified shown as below.

$$\mathbf{Z},\ \boldsymbol{y_1},\ \boldsymbol{y_2}\ \textbf{and}\ \boldsymbol{y_3}$$

Where Z represent the total cost of raw materials required

$y_1$represent the n-butane required per year

$y_2$represent the dibutyl phthalate solvent (DBP) required per year

$y_3$represent the vanadium phosphorus oxide catalyst (VPO) required per year

The algebraic equations including the constraints and objective function. The constraints involved in the optimization problem are listed as below.

$$y_1 \leq 24281$$
$$y_2 \leq 500000$$
$$y_3 \leq 45000$$

$$y_1, y_2, y_3 \geq 0$$

Objective function:

$$\text{Minimize Z} = 3.92\, y_1 + 247.8\, y_2 + 16.76\, y_3$$

By using GAMS algebraic modelling language, the algebraic equations listed above are coded accordingly in GAMS as shown in Figure 2.2.4.

```
Variables Z;

Positive Variables y1, y2, y3;

Equations OBJ, butane, DBP, VPO;

OBJ..       Z  =E= 3.92*y1 + 247.8*y2 + 16.76*y3;
butane..    y1 =G= 24821;
DBP..       y2 =G= 500000;
VPO..       y3 =G= 45000;

Model  rawmaterialproblem /all/ ;

Solve rawmaterialproblem USING LP MINIMIZING Z;

Display y1.L, y2.L, y3.L, Z.L;
```

Figure 2.2.4: Model coding in GAMS

Based on the Figure 2.2.4, all the variables are declared in GAMS. The objective function variable Z is declared as the 'Variables', while the decision variables are declared as 'Positive Variables'. Next, all the algebraic equations are listed down using 'Equations'. In this optimization case, the model named as rawmaterialproblem is utilized. The model specified 'all' indicates that all the previously defined constraints are to be included in this model. To solve the model rawmaterialproblem, Linear Programming (LP) is chosen as solution procedure to minimize the objective function, hence the command using LP Minimizing Z is used. Finally, by using 'Display y1.L, y2.L, y3.L, Z.L', the model coding was done, and the model is going to run. Then, the summary of optimal decision variables and the minimized objective function was obtained as shown in Figure 2.2.5.

```
--- LP status (1): optimal.
--- Cplex Time: 0.03sec (det. 0.00 ticks)


Optimal solution found
Objective:    124751498.320000


                          LOWER          LEVEL          UPPER         MARGINAL

---- EQU OBJ                .              .              .             1.0000
---- EQU butane        24821.0000     24821.0000        +INF            3.9200
---- EQU DBP          500000.0000    500000.0000        +INF          247.8000
---- EQU VPO           45000.0000     45000.0000        +INF           16.7600

                          LOWER          LEVEL          UPPER         MARGINAL

---- VAR Z                -INF      1.2475150E+8        +INF             .
---- VAR y1                 .          24821.0000        +INF             .
---- VAR y2                 .         500000.0000        +INF             .
---- VAR y3                 .          45000.0000        +INF             .


**** REPORT SUMMARY :        0     NONOPT
                             0 INFEASIBLE
                             0  UNBOUNDED
GAMS 42.5.0  cf11b917 Mar 30, 2023          WEX-WEI x86 64bit/MS Windows - 04/22/23 13:17:13 Page 7
G e n e r a l   A l g e b r a i c   M o d e l i n g   S y s t e m
E x e c u t i o n


----      16 VARIABLE y1.L                 =    24821.000
             VARIABLE y2.L                 =   500000.000
             VARIABLE y3.L                 =    45000.000
             VARIABLE Z.L                  = 1.247515E+8
```

Figure 2.2.5: Optimized Values shown by GAMS.

According to Figure 2.2.5, the minimized solution of RM 124,751,500.00 for objective function is obtained from GAMS. The optimized amounts of raw materials required per year including n-butane (y_1), dibutyl phthalate solvent (DBP) (y_2) and Vanadium phosphorus oxide catalyst (VPO) (y_3) are 24821 kg/year, 500000 kg/year and 45000 kg/year respectively.

<u>Brief Comparison of Results from Microsoft Excel and GAMS & Conclusion.</u>

Both Microsoft Excel Solver and GAMS result in the optimized amounts of raw materials required per year including n-butane (y_1), dibutyl phthalate solvent (DBP) (y_2) and Vanadium phosphorus oxide catalyst (VPO) (y_3) are 24821 kg/year, 500000 kg/year and 45000 kg/year respectively. Microsoft Excel Solver result in a minimized solution of RM 124,751,498.30, while GAMS give a rounded number which is RM 124,751,500.00. However, but substituting all the values the optimized decision variables given by GAMS into the objective function including $\boldsymbol{y_1}$**,** $\boldsymbol{y_2}$ **and** $\boldsymbol{y_3}$**,** the minimized solution of RM 124,751,498.30 can be obtained. Hence, all the variable values are said to be the same. The values obtained for each variable from both Microsoft Excel Solver and GAMS are tabulated in Table 2.2.3.

Table 2.2.3: Comparison result obtained from Microsoft Excel Solver and GAMS.

Variables	**Cost (RM)**	y_1 **(kg/year)**	y_2 **(kg/year)**	y_3 **(kg/year)**
Solver's Solution	124,751,498.30	24821	500000	45000
GAMS' Solution	124,751,500.00	24821	500000	45000

The optimization problem was successfully solved using both Microsoft Excel Solver and GAMS, with identical variable values obtained fulfilling the constraints and resulting in the minimized annual cost of raw materials required. Therefore, both software is considered good solvers for linear programming problems as they give the same optimal results. However, Microsoft Excel Solver has limitations when it is used to solve linear or non-linear problems with more than 200 decision variables as decision variables are limited in Solver. In addition, it has limitations to solve linear or non-linear problems over 100 constraints which make it challenging to solve complex models.

On the other hand, GAMS is more difficult to understand due to its unique coding language, but it is a safer option due to its ability to set constraint names for better recognition. GAMS has a lower tendency to generate different solutions as compared to Microsoft Excel SOLVER which is more sensitive to its initial values of the manipulated cells. Hence, when dealing with large and complex models, GAMS is more preferred to be used due to its unique language and ability to handle more than 100 constraints. For the small and simple models such as profit calculation and raw material optimization, Microsoft Excel solver is a more user-friendly option.

2.3 Refinery Planning and Scheduling (Khadija Nadim)

Introduction and Description of the Problem

Planning and scheduling are both important aspects of management in any industry. Planning refers to the manufacturing capacity of the plant under constraints of resources, costs, demands and the like. While scheduling refers to the details of material flow, manufacturing, and production of resources. Planning and scheduling are viewed as distinct levels in the manufacturing hierarchy as shown, but often a fair amount of overlap exists between the two. The time scale can often be the determining factor in whether a given problem is a planning or scheduling one: planning is typified by a time horizon of months or weeks, whereas scheduling tends to be of shorter duration, that is, weeks, days, or hours, depending on the cycle time from raw materials to final product (Edgar et al., 2001).

Problem Statement and Formulation of Objective Function.

Consider a refinery that produces four different types of products, namely, gasoline, heating oil, jet fuel and lube oil. There are 4 crudes required to produce these oils namely x1, x2, x3 and x4 in the fuel chain process. X5 is the amount of crude x4 that is used in the lube chain process. The yields of the oils produced by each of these crudes are given below in figure 2.3.1. The objective of the function is to maximize the profit per week by allocating each crude between the two processes subject to supply and demand.

The objection junction becomes, sum of the total income each crude brings in per week minus the total costs per week.

Maximize Z (Profit) = $\sum_{p=1}^{4} v_p\, Q_p - \sum_{c=1}^{5} C_c\, x_c$

where, p = Product fuels (p = 1,2,3,4)
c = identification of crude (c = 1,2,3,4,5)
v = selling price of the fuels ($/barrel)
Q_p = Production of each fuel (kbarrel/week)
C_c = Total cost of a crude per week ($/week)
x_c = amount of each crude used in production of fuel (barrel crude)

Description of Data

	Product Yields (barrel/barrel crude)				
Products (p)	**Fuel Chain (Crude)**				**Lube Chain**
	1	**2**	**3**	**4**	**4**
Gasoline	0.6	0.5	0.3	0.4	0.4
Heating oil	0.2	0.2	0.3	0.3	0.1

Jet fuel	0.1	0.2	0.3	0.2	0.2
Lube oil	0.0	0.0	0.0	0.0	0.2

Table 2.3.1: Product yields. Source: (Edgar et al., 2001).

The selling price of gasoline, heating oil, jet fuel and lube oil are 45, 30, 15 and 60 $/barrel respectively. Moreover, the Crude costs in $/barrel and operating cost in $/barrel are given below.

Crude	**1**	**2**	**3**	**4**	**5**
Crude cost	15	15	15	25	25
Operating Cost	5	8.5	7.5	3	2.5

Table 2: Cost Breakdown. Source: (Edgar et al., 2001).

The amount of each fuel produced is calculated by obtaining the yield of a fuel from a crude (a_{pc}) and multiplying it with the amount of each crude used (x_c). The sum of all the crudes required to make up the fuel is added to obtain the final production amount.
$Q_p = a_{p1} * x_1 + a_{p2} * x_2 + a_{p3} * x_3 + a_{p4} * x_4 + a_{p5} * x_5$ (p = 1,2,3,4)

For example, the total production of gasoline fuel is given by,
$Q_1 = a_{11} * x_1 + a_{12} * x_2 + a_{13} * x_3 + a_{14} * x_4 + a_{15} * x_5$
$Q_1 = 0.6 * x_1 + 0.5 * x_2 + 0.3 * x_3 + 0.4 * x_4 + 0.4 * x_5$

The total cost of the fuel is the sum of the crude cost and operating costs of a crude and multiplying it with the amount of crude used (x_c). For example, the crude cost and operating costs of gasoline are given as 15$ and 5$ respectively. Hence the cost is given by C_c = $20 and the total cost per week would be $20 * x_1$.

The constraints are, given as,
The amount of each fuel produced per week should be less than the demand, $Q_p \leq D_p$. The demand for gasoline, heating oil, jet fuel and lube oil are 170, 85, 85 and 20 kbarrel/week respectively.

The amount of crude used cannot exceed the amount supplied to the manufacturer, $x_c \leq S_c$ (c=1,2,3). The amount of crude 1, 2 and 3 supplied are 100 kbarrel/week (S_c). The amount of crude 4 supplied that is to be used in both fuel chain and lube chain process is 200 kbarrel/week. Therefore, the constraint is written as, $x_4 + x_5 \leq 200$.

Moreover, the non-negativity constraints are as follows,
$Q_p \geq 0$ (p = 1,2,3,4)
$x_c \geq 0$ (c = 1,2,3,4,5)

Solution from Excel
The solution is obtained by making a table in excel as given in Figure 1 below. The equations for production and total cost are entered as explained above. The cell 4+5 is added to satisfy the constraint of $x_4 + x_5 \leq 200$ with regards to the available supply of crude 4.

	Product Yield (bbl/bbl crude)								
	Crude				Lube Chain		Selling Price, v	Production, Qp	Demand
Products	1	2	3	4	5	4+5	($/bbl)		(1000 bbl/week)
Xc	100	100	66.66667	0	100	100			
Gasoline (P1)	0.60	0.50	0.30	0.40	0.40		45.00	170	170
Heating Oil (P2)	0.20	0.20	0.30	0.30	0.10		30.00	70	85
Jet Fuel (P3)	0.10	0.20	0.30	0.20	0.20		15.00	70	85
Lube Oil (P4)	0.00	0.00	0.00	0.00	0.20		60.00	20	20
Income/week	3450.00	3150.00	1800.00	0.00	3600.00				
Crude Cost ($/bbl)	15.00	15.00	15.00	25.00	25.00				
Operating Cost ($/bbl)	5.00	8.50	7.50	3.00	2.50				
Total Cost ($/bbl)	2000.00	2350.00	1500.00	0.00	2750.00				
							Z (Profit)		
Profit/week	1450.00	800.00	300.00	0.00	850.00		3400.00		
Avaliable (1000 bbl/week)	100.00	100.00	100.00	200.00					

Figure 2.3.1: Results from Solver

The constraints for supply and demand are added into the solver. The total profit is maximized, and the unconstrained variables are non-negative. Simplex Linear programming algorithm is utilized to solve the model.

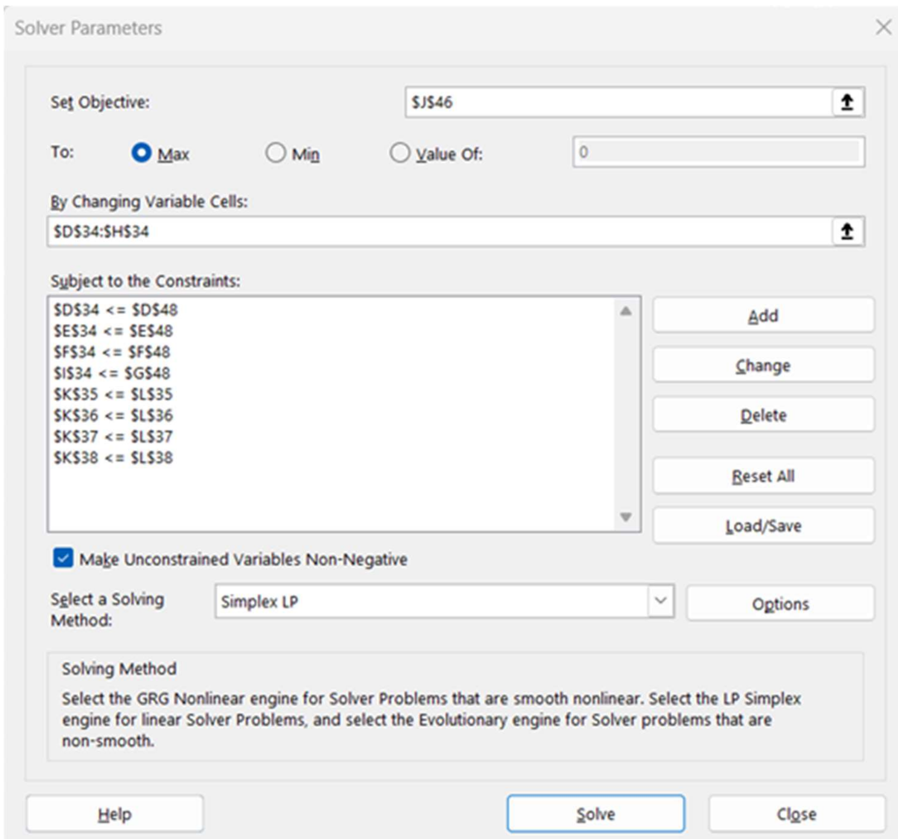


Figure 2.3.2: Solver Input Values

As seen in figure 1, the total profits per week were optimized to be 3400$. All of the available crude 1 and 2 were utilized. Only 66.67 barrels of crude 3 wa s used, and 100 barrels of crude 4 were used in the lube chain process while none was used in the fuel chain process. The quantities of fuels produced were as follows: 170 barrels/week of gasoline, 70 barrels/week of heating oil and jet fuel and 20barrels/week of lube oil.

Justification of Selection

The model was solved with excel solver as it was a simpler approach to solver the linear problem. All of the identifying variables and values could easily be recognized and tabulated in a more organized method. Moreover, the problem was a simple linear model, excel can easily provide an accurate result. The model was solved in excel due to the ease in which other functions could be utilized such as the addition of total cost. While in GAMS this would have to be done manually to provide a clear and concise result.

2.4 Optimizing Labor Scheduling to Minimize Labor Cost in Production of Maleic Anhydride (Al-Rawi and Mukherjee, 2019) (Wong Pei Yu)

Introduction and Description of the Problem

In maleic anhydride production, a significant number of labor workers are necessary to operate the process plant, resulting in high labor costs. As a result, optimizing the number of hired workers is crucial to minimize these expenses. In the past, labor scheduling was often created using tools such as Microsoft Word and Excel, or through pen-and-paper methods for small and medium-sized enterprises with limited computer software and cost resources. Scheduling optimization can be widely applied across various industries, such as scheduling airlines to optimize flight routes and minimize fuel consumption, scheduling staff in hotels, nurses in hospitals, or labor in production sites.

Utilizing workforce scheduling optimization can increase profits by determining the best workforce schedule to minimize labor costs. Labor costs are the total expenses paid by employers for employee employment, including direct labor costs for workers in production, indirect labor costs for non-production employees, fixed labor costs that remain unchanged for a period, and variable labor costs that fluctuate with production demands. During peak seasons, manufacturing companies may hire variable labor to meet production demand. By reducing labor costs, overall production expenses can decrease, leading to increased company profits.

In a typical manufacturing plant, various workers are necessary, including production workers to operate machines and pack goods, engineers to design and monitor product quality, electricians to repair faulty equipment that involve wiring, control systems and electrical power systems and drivers to transport finished goods.

Problem Statement and Formulation of Objective Function.

In this scenario, the optimization of workforce scheduling in a maleic anhydride manufacturing plant is the objective. Table 2.4.1 displays the available workforce during each shift. Assuming a 25-day work month, the daily wage for each type of workforce can be calculated using Equation 2.4.1. Production workers' monthly salary is assumed to be RM1500, while engineers receive RM3600 and electricians and drivers receive RM2200 each per month.

$$Wage\ per\ day = \frac{Monthly\ Salary}{25\ working\ days} \ldots\ldots (Equation\ 2.4.1)$$

The workforce is assumed to work 6 days a week in two shifts, morning and evening, to ensure 24-hour operation. Each cell in the schedule represents the availability of a specific workforce during a particular shift, with 1 indicating that they are required to work and 0 indicating that they are not needed. For instance, if $X_{1,1,S1} = 1$, all production workers will be working on day 1 shift 1, while $X_{3,3,S1} = 0$ means that no electricians will be working on day 3 shift 1.

The scheduling of working shifts is based on specific reasons. Production workers must be available for every shift every working day to ensure continuous manufacturing. Engineers work for three shifts continuously and then take one shift off to monitor and prepare for potential quality issues. Electricians take one shift off for every two days, alternating between morning and evening shifts. This is because the engineer on duty can handle any issues that arise and wait for the electrician to repair the problem during the next available shift. Lastly, drivers only need to work the evening shift, as most products are only ready for manufacturing and packing in the afternoon.

Table 2.4.1: Workforce Available Per Shift

Wage/Day, C_i (RM/day)	Workforce, X_i	Day 1		Day 2		Day 3		Day 4		Day 5		Day 6	
		S1	S2	S1	S2	S1	S2	S1	S2	S1	S2	S1	S2

60	**Production Worker**	1	1	1	1	1	1	1	1	1	1	1	1
144	**Engineer**	1	1	1	0	1	1	1	0	1	1	1	0
88	**Electrician**	1	0	1	1	0	1	1	1	1	0	1	1
88	**Driver**	0	1	0	1	0	1	0	1	0	1	0	1
Workforce available per shift		92	91	90	86	88	95	90	87	94	92	93	87

Description of Data to be Used In the Case Study.

The objective function of this case is to minimize the cost of labor per shift. The equation for calculating labor cost is shown in Equation 2.4.2, where C_i represents the daily wage for each category of workforce and X_{i-} represents the number of workers. Daily wage is used instead of wage per shift because no worker will be working for two consecutive shifts. The objective function is represented by Equation 2.4.3, where the labor cost is denoted by C, and the daily wages are substituted.

Algebraic Equations

Objective function:

$$Labor\ Cost, C = \sum_{i=1}^{4} C_i X_i \ \ldots\ldots (Equation\ 2.4.2)$$

$$Minimize\ C = 60X_1 + 144X_2 + 88X_3 + 88X_4 \ \ldots\ldots (Equation\ 2.4.3)$$

Decision variables:

$X_1 = Number\ of\ production\ workers$

$X_2 = Number\ of\ engineers$

$X_3 = Number\ of\ electricians$

$X_4 = Number\ of\ drivers$

Constraints:

$$X_1 + X_2 + X_3 \geq 92\ (Day\ 1\ Shift\ 1)$$

$$X_1 + X_2 + X_4 \geq 91\ (Day\ 1\ Shift\ 2)$$

$$X_1 + X_2 + X_3 \geq 90\ (Day\ 2\ Shift\ 1)$$

$$X_1 + X_3 + X_4 \geq 86\ (Day\ 2\ Shift\ 2)$$

$$X_1 + X_2 \geq 88\ (Day\ 3\ Shift\ 1)$$

$$X_1 + X_2 + X_3 + X_4 \geq 95\ (Day\ 3\ Shift\ 2)$$

$$X_1 + X_2 + X_3 \geq 90\ (Day\ 4\ Shift\ 1)$$

$$X_1 + X_3 + X_4 \geq 87\ (Day\ 4\ Shift\ 2)$$

$$X_1 + X_2 + X_3 \geq 94\ (Day\ 5\ Shift\ 1)$$

$$X_1 + X_2 + X_4 \geq 92\ (Day\ 5\ Shift\ 2)$$

$$X_1 + X_2 + X_3 \geq 93\ (Day\ 6\ Shift\ 1)$$

$$X_1 + X_3 + X_4 \geq 87\ (Day\ 6\ Shift\ 2)$$

Minimum workforces required per shift:

$$X_1 \geq 50\ ;\ X_2 \geq 20\ ;\ X_3 \geq 7\ ;\ X_4 \geq 5$$

Positive variables:

$$X_1,\ X_2,\ X_3\ ,\ X_4 \geq 0$$

<u>Solutions from GAMS</u>

The GAMS code for the model is presented in Figure 2.4.1. Initially, the variable C, which represents the labor cost, is declared, followed by declaring X1, X2, X3, and X4 as positive variables, as the number of workforces cannot be negative, fractions or decimals. The objective function and constraints are then inputted. The optimization problem involves a total of one objective function and 16 constraints. A mixed-integer programming technique is used to solve this problem, and the optimal solutions can be displayed using the 'display' keyword. The optimum solutions obtained are presented in Figure 2.4.2.

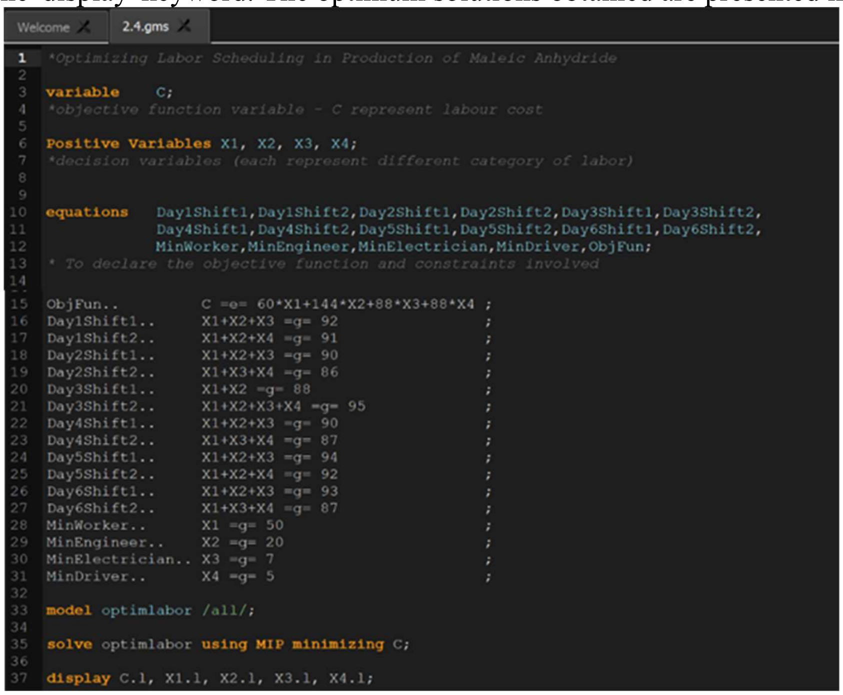


Figure 2.4.1: Model Coding in GAMS

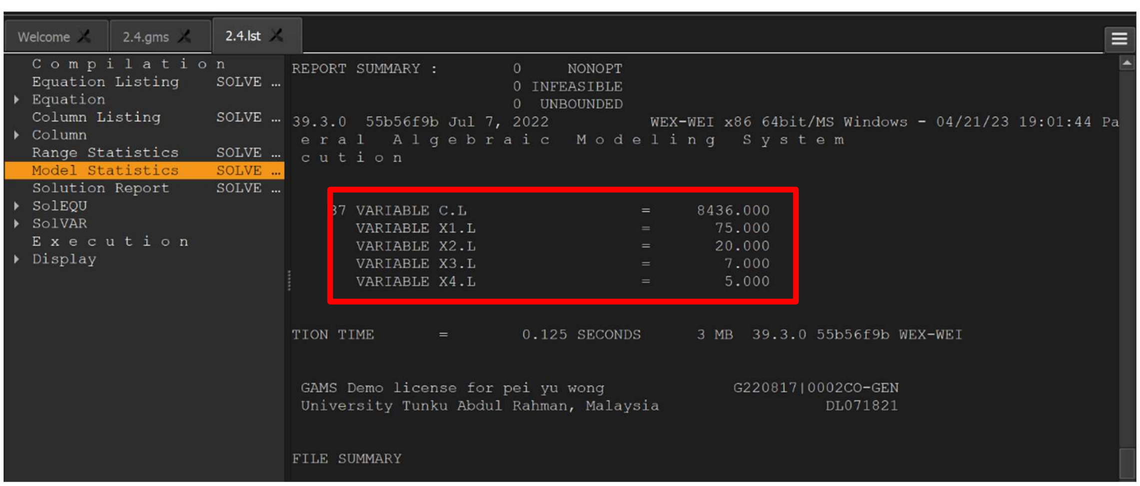


Figure 2.4.2: Optimum Results

From the results, the minimum labour cost of one shift is RM8436 when 75 production workers, 20 engineers, 7 electricians and 5 workers are allocated every shift. A total of 107 labor are required during one shift to ensure the work environment runs efficiently while minimizing labor expenses.

<u>Justification of Selection</u>

The selection of GAMS software over Microsoft Excel in this optimization problem is justified due to this case involves multiple variables and constraints, which has a large amounts of data and makes it complex. GAMS is designed to handle such complex optimization problems efficiently and provide optimal solutions in a relatively shorter time. Besides, GAMS provides specialized optimization algorithms that are specifically designed to solve optimization problems. These algorithms can provide better and more efficient solutions than the optimization algorithms available in Excel. Compared to Microsoft Excel Solver Function, it only provides three solving methods which are GRG nonlinear, simplex LP and evolutionary. GAMS has an error checking feature that will halt the system when an error is detected. The error will be highlighted in red, and a helpful comment will be displayed to assist in correcting the mistake. Excel is a general-purpose spreadsheet program while GAMS provides a more intuitive and user-friendly interface for modelling and solving optimization problems.

2.5 Optimizing Chemical Production of Maleic Anhydride in Mosanto (Tham Ting Woon)

(a) Introduction and Description of Problem

A chemical production of maleic anhydride had been developed in Monsanto. Monsanto is a large production in producing maleic anhydride. It involves the oxidation of n-butane to produce maleic anhydride. This reaction is carried out in a fixed bed reactor using vanadium-phosphorus oxide catalyst. It is an exothermic reaction. Butane is converted into maleic anhydride using catalytic oxidation. The compressor in the process is used to provide ambient air to the fixed bed reactor. Butane is mixed with the air and will feed into the reactor. The gas that exits through the reactor is cooled down by circulating a cooling fluid and will carry out absorption and distillation to get the desired purity of maleic anhydride. The byproduct of gas is used as a fuel for steam production. The production process involves several steps and each of them has its own set of variables and constraints.

Maleic anhydride has many uses. It can be used in unsaturated polyester resins in manufacturing boat hulls, counter tops and so on. Maleic anhydride is also used in oil additives and agricultural chemicals.

The production yield is determined by a few variables such as the raw material feed rate, reactor velocity, reactor pressure, catalyst factor, purification factor and process age factor. In this case, linear programming is used to find the optimal values of variables that maximize the yield of maleic anhydride.

(b) Problem statement and formulation of objective function.

In this case study, the yield is determined by the raw materials feed rate, reactor velocity, reactor pressure, catalyst factor, purification factor and process age factor. But maximizing the production will cause low yield and maximizing yield will result in low production. Hence, an optimization model was developed to find the optimal solution that can maximize the yield.

Discrete linear programming had been applied as the solution for this case. The ranges and value of the variables are different for each reactor. However, the value of catalyst, purification and process age are the same for a reactor along its operating levels.

The problem statement in this case study describes the production process of maleic anhydride, where the objective function is to maximize the yield of product by changing the variables.

Objective Function:

$$Yield = \left(\frac{AB}{C}\right) \times DE \times \frac{1}{F}$$

Where;

A= raw material feed rate

B= reactor velocity

C= reactor pressure

D= catalyst factor

E= purification factor

F= process age factor

(c) Presentation and description of data to be used in the case study

Table 2.5.1: Range of Variables

Variables	Low Level	Upper Level
A (raw material feed rate)	150	250
B (reactor velocity)	2	10
C (reactor pressure)	50	100
D (catalyst factor)	0	5
E (purification factor)	-	1
F (process age factor)	0	10

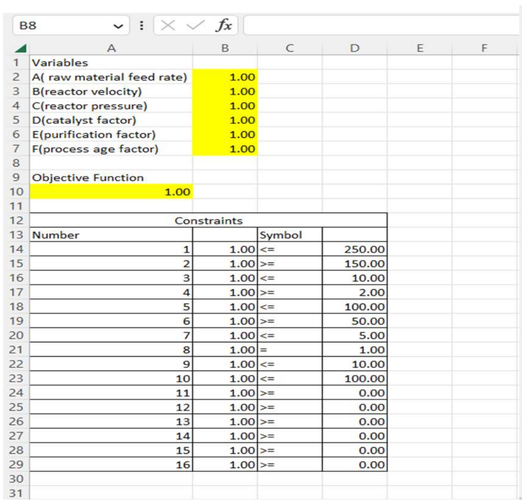
Table 2.5.1 shows the value range of variables A, B, C, D, E and F in maleic anhydride production. The upper limit and lower limit of the variables are listed down. The formulation of constraints can be done once the decision variables are confirmed. During the process of production of maleic anhydride, the feed rate of raw materials which is n-butane is between 150 kg/h to 250 kg/h (Boykin,2012). The velocity of the gas stream through the reactor is between 2 m/s and 10 m/s. The reactor pressure is between 50 kPa to 100 kPa. The catalyst factor is 0 to 5, purification factor should equal to one while the process age factor should in between 0 to 10. All the constraints are non-negativity. The data above are used to determine the optimal value of raw materials feed rate, reactor velocity and reactor pressure that maximize the yield of maleic anhydride. The constraints of this case are as below:

Subject to:

$$150 \leq A \leq 250$$
$$2 \leq B \leq 10$$
$$50 \leq C \leq 100$$
$$0 \leq D \leq 5$$
$$E = 1$$
$$0 \leq F \leq 10$$

(d) Solution from Microsoft Excel

(i) Print Screen of Spreadsheet and description of Solver Step



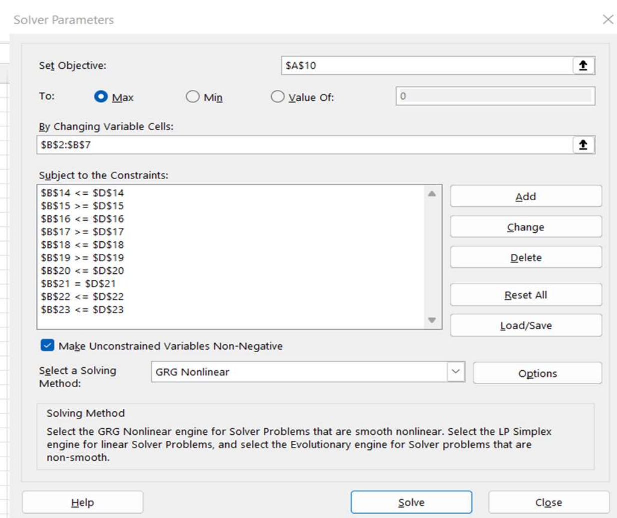


Figure 2.5.1: Details that Type into Microsoft Excel

Figure 2.5.2: Details of Set Objective, Changing Variables Cell and Constraints are added into Solver Parameter

Figure 2.5.1 and 2.5.2 show the print screen of spreadsheet from Microsoft Excel. The values for each cell are filled based on the values in the articles. Initially, the value of A, B, C, D, E and F at cell B2 until B7 can be any value. In this case, the value is 1.

The objective function which is at cell A10 is calculated based on the equation.

$$Yield = \left(\frac{AB}{C}\right) \times DE \times \frac{1}{F}$$

The value of objective function before solver is equal to 1. Next, the constraints are typed into Microsoft Excel. All the constraints are non-negativity constraints that are shown in cell B24 until B29. The limit of raw material feed rate is in between 150 kg/h to 250 kg/h, reactor velocity is in between 2 m/s to 10 m/s, reactor pressure in between 50 kPa to 100 kPa. Catalyst factor should be less than or equal to 5, purification factor should be equal to one while process age factor should be less than or equal to 10.

To solve this case using solver function in Microsoft Excel, Solver can be found under "Data". After clicking the solver, a pop-out window will appear as Figure 2.5.2. Under "Set Objective:", cell ($A$10) is selected for objective function. Next, "Max" is selected to maximize the yield. Under the section of "By Changing Variables Cell, cells at B2 until B7 are selected. Under the section "Subject to the Constraints:", cell B14 until B23 are selected based on their symbol, upper limit, and lower limit respectively. Tick '✓' at the box "Make Unconstraint Variables Non-Negative. The solving method in this case is GRG Nonlinear. Next, click the "Solve" button where the optimal solution will be solved by Solver Function.

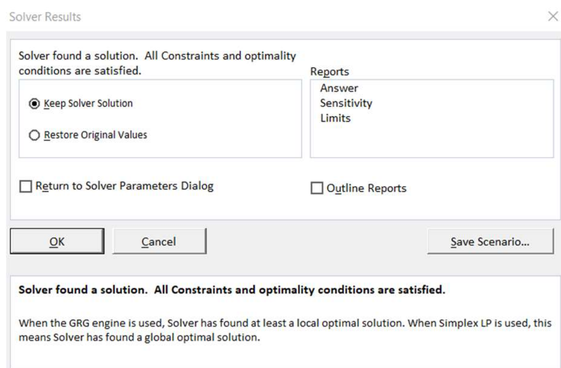
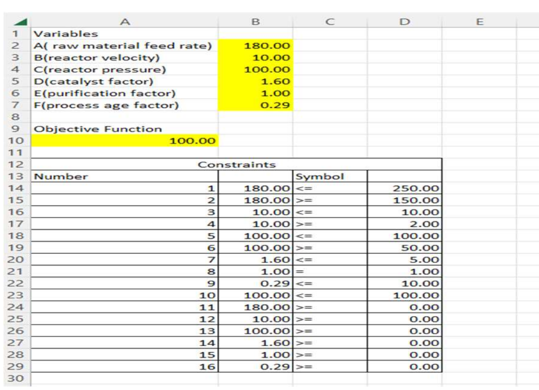


Figure 2.5.3: Pop out window after clicking Solve button

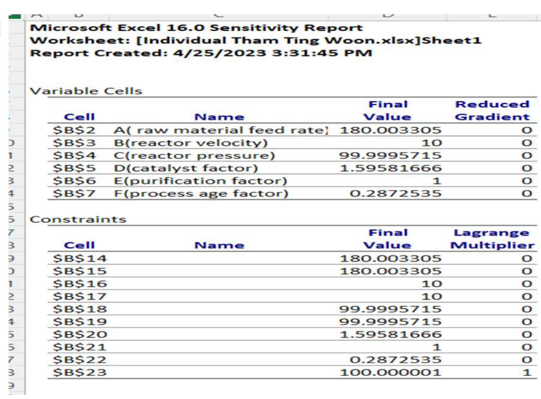
After clicking "Solve" button, a pop out window as Figure 2.5.3 will be shown. "Solver found a solution. All constraints and optimality conditions are satisfied" means that this problem had been successfully solved by solver function by the given constraints. All the value from B2 until B7 will change to maximize the yield at cell A10. Furthermore, under the "Reports" section, the answer report, sensitivity report and limit report can be generated by Microsoft Excel in the new spreadsheet.

(ii) Optimum results obtained



	A	B	C	D	E
1	Variables				
2	A(raw material feed rate)	180.00			
3	B(reactor velocity)	10.00			
4	C(reactor pressure)	100.00			
5	D(catalyst factor)	1.60			
6	E(purification factor)	1.00			
7	F(process age factor)	0.29			
8					
9	Objective Function				
10	100.00				
11					
12	Constraints				
13	Number		Symbol		
14	1	180.00	<=	250.00	
15	2	180.00	>=	150.00	
16	3	10.00	<=	10.00	
17	4	10.00	>=	2.00	
18	5	100.00	<=	100.00	
19	6	100.00	>=	50.00	
20	7	1.60	<=	5.00	
21	8	1.00	=	1.00	
22	9	0.29	<=	10.00	
23	10	100.00	<=	100.00	
24	11	180.00	>=	0.00	
25	12	10.00	>=	0.00	
26	13	100.00	>=	0.00	
27	14	1.60	>=	0.00	
28	15	1.00	>=	0.00	
29	16	0.29	>=	0.00	
30					

Figure 2.5.5: Optimal results solved by Solver Function



Microsoft Excel 16.0 Sensitivity Report
Worksheet: [Individual Tham Ting Woon.xlsx]Sheet1
Report Created: 4/25/2023 3:31:45 PM

Variable Cells

Cell	Name	Final Value	Reduced Gradient
$B$2	A(raw material feed rate)	180.003305	0
$B$3	B(reactor velocity)	10	0
$B$4	C(reactor pressure)	99.9995715	0
$B$5	D(catalyst factor)	1.59581666	0
$B$6	E(purification factor)	1	0
$B$7	F(process age factor)	0.2872535	0

Constraints

Cell	Name	Final Value	Lagrange Multiplier
$B$14		180.003305	0
$B$15		180.003305	0
$B$16		10	0
$B$17		10	0
$B$18		99.9995715	0
$B$19		99.9995715	0
$B$20		1.59581666	0
$B$21		1	0
$B$22		0.2872535	0
$B$23		100.000001	1

Figure 2.5.4: Optimal results from Sensitivity Report

Microsoft Excel 16.0 Limits Report
Worksheet: [Individual Tham Ting Woon.xlsx]Sheet1
Report Created: 4/25/2023 3:31:58 PM

	Objective	
Cell	Name	Value
$A$10	Objective Function	100.00

	Variable		Lower	Objective	Upper	Objective
Cell	Name	Value	Limit	Result	Limit	Result
$B$2	A(raw material feed rate)	180.00	150.00	83.33	180.00	100.00
$B$3	B(reactor velocity)	10.00	2.00	20.00	10.00	100.00
$B$4	C(reactor pressure)	100.00	100.00	100.00	100.00	100.00
$B$5	D(catalyst factor)	1.60	0.00	0.00	1.60	100.00
$B$6	E(purification factor)	1.00	1.00	100.00	1.00	100.00
$B$7	F(process age factor)	0.29	0.29	100.00	10.00	2.87

Figure 2.5.6: Optimal results from Limit Report

Microsoft Excel 16.0 Answer Report
Worksheet: [Individual Tham Ting Woon.xlsx]Sheet1
Report Created: 4/25/2023 4:08:38 PM
Result: Solver found a solution. All Constraints and optimality conditions are satisfied.
Solver Engine
Engine: GRG Nonlinear
Solution Time: 0.219 Seconds.
Iterations: 9 Subproblems: 0
Solver Options
Max Time Unlimited, Iterations Unlimited, Precision 0.000001
Convergence 0.0001, Population Size 100, Random Seed 0, Derivatives Central
Max Subproblems Unlimited, Max Integer Sols Unlimited, Integer Tolerance 1%, Assume NonNegative

Objective Cell (Max)

Cell	Name	Original Value	Final Value
$A$10	Objective Function	1.00	100.00

Variable Cells

Cell	Name	Original Value	Final Value	Integer
$B$2	A(raw material feed rate)	1.00	180.00	Contin
$B$3	B(reactor velocity)	1.00	10.00	Contin
$B$4	C(reactor pressure)	1.00	100.00	Contin
$B$5	D(catalyst factor)	1.00	1.60	Contin
$B$6	E(purification factor)	1.00	1.00	Contin
$B$7	F(process age factor)	1.00	0.29	Contin

Figure 2.5.7: Optimal results from Answer Report

The value at cell B2 until B7 and A10 will change accordingly to maximize the yield. In this case, Solver found that the raw materials feed rate (A) should be at 180 kg/h. The value of reactor velocity (B) is at 10 m/s, the reactor pressure (C) is at 100 kPa, catalyst factor (D) at 1.60, purification factor (E) equal to one and process age factor (F) at 0.29 to maximize the yield at 100 %.

(e) **Justification of Selection**

The reason to choose Microsoft Excel Solver Function to solve this problem instead of using GAMS is because Excel Solver is easy to use optimization tool. It does not require professional skills to operate it. It does not require programming knowledge, making it accessible for a wider range of users. Besides, it is already installed on our computer and many people are already familiar with Excel, it is more accessible than GAMS. Excel Solver is free to add into Excel so there is no need to purchase or install any additional software. In this case study, the optimization problem is small, and it can be easily solved by using Excel Solver. Furthermore, Excel Solver is more flexible in solving the optimization problems. It can handle a wide range of optimization problems such as linear, nonlinear and integer programming problems. Excel Solver also provides a tool for visualizing the problems and its solution easily, making the users understand and interpreting the results more easily.

3 REFERENCES

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