Supplementary Information (SI) for RSC Sustainability.

Supplementary Information

Case Study 1:

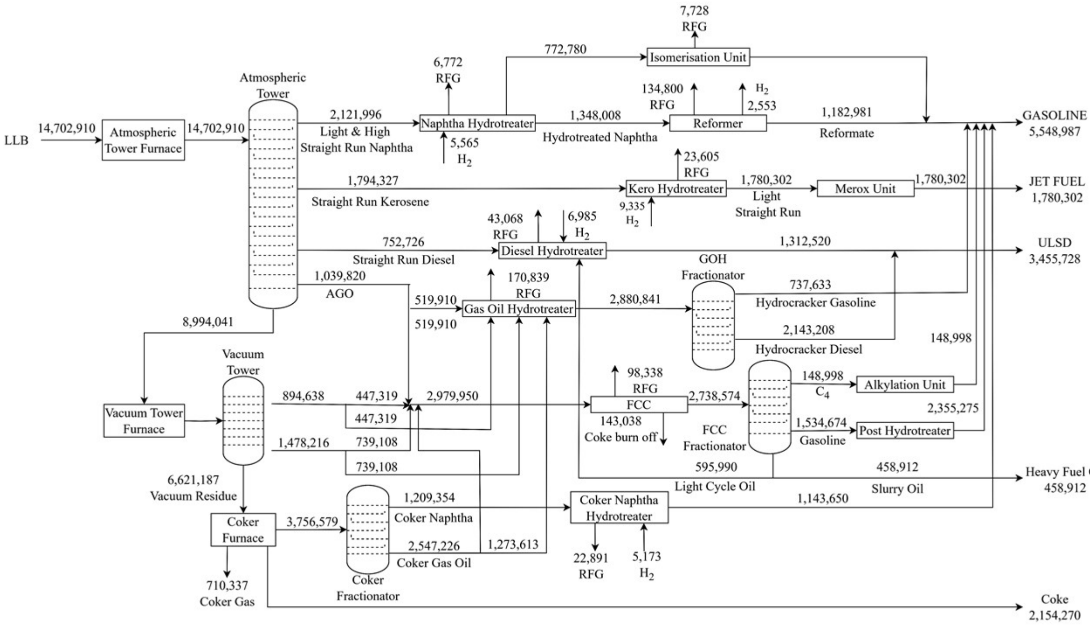

Figure S1:Process flow in a traditional deep configuration refinery (Reproduced from Bhuiyan, *et al.*[26] with permissions)

Table S1: Economic factor and carbon intensity of utilities

Utility	Economic Factor	Unit	Source	Carbon Factor	Unit	Source
Electricity	0.10	USD/kWh	Yap, *et al.*[20]	184.8	g CO_2/MJ	Abella, *et al.*[27]
Steam	0.012	USD/kg		75.4	g CO_2/MJ	
Natural Gas	0.0027	USD/MJ	Bhuiyan, *et al.*[26]	69.2	g CO_2/MJ	
Hydrogen	0.0034	USD/MJ		81.7	g CO_2/MJ	
Cooling Water	0.00054	USD/MJ	Yap, *et al.*[20]	77.7	g CO_2/MJ	Yap, *et al.*[20]
Refrigerant	0.79	USD/MJ	Daikin[28]	11.96	g CO_2/MJ	Daikin[28]

Table S2: Refinery process shared and dedicated facilities

Shared facility	Dedicated facility
Desalter	Naphtha hydrotreater
Atmospheric tower	Coker naphtha hydrotreater
Vacuum tower and furnace	Fluid catalytic cracking post hydrotreater
Gas oil hydrotreater (GOH) and fractionator	Alkylation unit
Coker furnace and fractionator	Catalytic naphtha reformer
Coker	Isomerisation unit
Fluid catalytic cracker (FCC) and main fractionator	Kerosene hydrotreater and merox unit
Fuel gas treatment and sulphur recovery	Diesel hydrotreater

Table S3: Refinery process energy inputs and outputs

Process Energy Inputs and Outputs	Input					Output
Process Unit	Power consumption MJ/day	Total NG requirement kg/day	Medium-pressure steam kg/day	High-pressure steam kg/day	Total hydrogen requirement kg/day	Hydrogen production kg/day
Desalter	5,402	-	-	-	-	-
Atmospheric Tower Furnace	-	6,228,841	-	-	-	-
Atmospheric Tower	324,113	-	319,719	-	-	-
Vacuum Tower Furnace	-	2,183,895	-	-	-	-
Vacuum Tower	59,754	-	286,420	-	-	-
Naphtha Hydrotreater	124,253	1,692,457	41,748	-	5,844	-
Kerosene Hydrotreater	141,396	1,902,060	-	47,508	9,802	-
Kerosene Merox Unit	4,915	-	-	-	-	-
Gas Oil Hydrocracker	457,528	-	-	-	93,925	-
Gas Oil Hydrocracker Fractionator	129,732	-	-	539,947	-	-
Diesel Hydrotreater	103,984	1,396,090	-	34,938	7,334	-
Coker Furnace	-	5,894,084	-	-	-	-
Coker	232,661	-	-	-	-	-
Coker Fractionator	48,658	-	41,123	-	-	-
Coker Naphtha Hydrotreater	106,690	1,448,511	-	35,847	5,432	-
Fluid Catalytic Cracking Post Hydrotreater	93,919	1,227,098	35,501	-	4,232	-
Fluid Catalytic Cracker	50,042	-	-	-	-	-
Fluid Catalytic Cracker Main Fractionator	35,335	-	10,144	-	-	-
Alkylation Unit	22,240	-	109,800	-	-	-
Catalytic Naphtha Reformer	124,918	-	-	157,394	-	30,226
Isomerisation Unit	27,492	1,223,476	-	-	43	-
Fuel gas treatment and sulphur recovery	201,960	2,749,997	-	-766,690	-	-
Total	2,294,995	25,946,509	844,455	48,945	126,611	30,226

Table S4: Refinery process CO_2 emissions

Process CO_2 Emissions	Input				
Process Unit	Power consumption t CO_{2eq}/day	Total NG requirement t CO_{2eq}/day	Medium-pressure steam t CO_{2eq}/day	High-pressure steam t CO_{2eq}/day	Total hydrogen requirement t CO_{2eq}/day
Desalter	1.00	-	-	-	-
Atmospheric Tower Furnace	-	431.04	-	-	-
Atmospheric Tower	59.90	-	67.02	-	-
Vacuum Tower Furnace	-	151.13	-	-	-
Vacuum Tower	11.04	-	60.04	-	-
Naphtha Hydrotreater	22.96	117.12	8.75	-	60.66
Kerosene Hydrotreater	26.13	131.62	-	11.68	101.75
Kerosene Merox Unit	0.91	-	-	-	-
Gas Oil Hydrocracker	84.55	-	-	-	975.01
Gas Oil Hydrocracker Fractionator	23.97	-	-	132.72	-
Diesel Hydrotreater	19.22	96.61	-	8.59	76.13
Coker Furnace	-	407.87	-	-	-
Coker	43.00	-	-	-	-
Coker Fractionator	8.99	-	8.62	-	-
Coker Naphtha Hydrotreater	19.72	100.24	-	8.81	56.39
Fluid Catalytic Cracking Post Hydrotreater	17.36	84.92	7.44	-	43.93
Fluid Catalytic Cracker	9.25	-	-	-	-
Fluid Catalytic Cracker Main Fractionator	6.53	-	2.13	-	-
Alkylation Unit	4.11	-	23.02	-	-
Catalytic Naphtha Reformer	23.08	-	-	38.69	-
Isomerisation Unit	5.08	84.66	-	-	0.44
Fuel gas treatment and sulphur recovery	37.32	190.30	-	-188.46	43.93
Total	424.12	1,795.50	177.01	12.03	1,314.32

Strategy 1 – Natural gas combined heat and power (NG CHP)

From Table 4, the total electric needed is 2,294,995 MJ,

$$Power\ required = 2{,}294{,}995\ MJ \times \frac{1.1574 \times 10^{-5}\ MW}{1\ MJ} = 26.56\ MW$$

For NG CHP system, the heat available by generation of electrical. From Table A2, the power-to-heat ratio of the NG – CHP is 1.1,

$$Heat\ available = 26.56\ MW \div 1.1 = 24.15\ MW$$

The heat is then used to produce medium - pressure (MP) steam for the process. From Table A1 the heating value of MP steam is taken as 2.78 MJ/kg,

$$MP\ steam\ produce,\ D_{MP\ steam} = 24.15\ MW \times \frac{1\ MJ}{1.1574 \times 10^{-5}\ MW}$$
$$= 2{,}086{,}573\ MJ \div 2.78\ \frac{MJ}{kg} = 750{,}566\ kg\ steam$$

NG CHP system with the efficiency of 69%,

$$Total\ fuel\ required = (26.56 + 24.15)\ MW \div 0.69 = 73.49\ MW$$

$$NG\ required = 73.49\ MW \times \frac{1\ MJ}{1.1574 \times 10^{-5}\ MW}$$
$$= 6{,}349{,}577\ MJ \div 47.14\ \frac{MJ}{kg} = 134{,}696\ kg\ NG$$

From Table 2, the NG utility cost on 0.00265 USD/MJ NG,

$$Cost\ of\ NG = 6{,}349{,}577\ MJ\ NG \times 0.00265\ \frac{USD}{MJ\ NG} = 16{,}826\ USD$$

The produced electric and steam by the NG CHP system act as the saving cost from buying fresh utilities. From Table 2, the utility cost of electric and steam is 0.028 USD/MJ electric and 0.012 USD/kg steam,

$$Saving\ cost = Electric\ utility\ \&\ Steam\ utility$$
$$= \left(2{,}294{,}995\ MJ \times 0.028\ \frac{USD}{MJ\ electric}\right) + \left(750{,}566\ kg \times 0.012 \frac{USD}{kg\ steam}\right) = 73{,}267\ USD$$

$$Total\ saving\ cost = Saving\ cost - Cost\ of\ NG$$
$$= (73{,}267 - 16{,}826)\ USD = 56{,}441\ USD$$

The emissions from NG CHP system are the use of natural gas. From Table 2, the emissions factor of NG is 69.3 g CO_2/MJ NG,

$$NG\ emissions = 6{,}349{,}577\ MJ\ NG \times 69.2\ \frac{g\ CO_2}{MJ\ NG} = 439{,}390{,}728\ g\ CO_2$$

The electricity and steam produced by the NG CHP system reduces the indirect emissions. From Table 2, the emissions factor of electric and steam is 184.8 g CO_2/MJ electric and 75.4 g CO_2/MJ steam,

$$Reduction\ emissions = Electric\ utility\ \&\ Steam\ utility$$

$$= \left(2{,}294{,}995\ MJ\ electric \times 184.8\ \frac{g\ CO_2}{MJ\ electric}\right) + \left(2{,}086{,}573\ MJ\ steam \times 75.4\ \frac{g\ CO_2}{MJ\ steam}\right)$$

$$= 581{,}442{,}680\ g\ CO_2$$

$$Total\ reduction\ emissions = Reduction\ emissions - NG\ emissions$$

$$= (581{,}442{,}680 - 439{,}390{,}728)\ g\ CO_2 \times \frac{1\ t}{10 \times 10^6\ g}$$

$$= 142.05\ t\ CO_2$$

Follow to EPA[1] the average total installed cost of gas turbine is 859 USD/kW. With the required gas turbine capacity of 26.56 MW,

$$Total\ installed\ cost = 26.56\ MW \times \frac{1000\ kW}{1\ MW} \times 859\ \frac{USD}{kW}$$

$$= 22{,}815{,}040\ USD$$

As the cost is in year of 2002, with the Chemical Engineering Plant Cost Index (CEPCI) of 395.6 and take CE index of 789.2 on year 2023.[2] The actual total installed cost can be calculated by using formula below,[3]

$$Cost\ in\ year\ A = Cost\ in\ year\ B \times \left(\frac{CEPCI\ in\ year\ A}{CEPCI\ in\ year\ B}\right)$$

$$Tota\ installed\ cost_{2023} = 22{,}815{,}040\ USD \times \left(\frac{789.2}{395.6}\right) = 45{,}514{,}736\ USD$$

The total installed cost is then converted to annualised capital cost (CAPEX) with multiply the annual capital charge ratio (ACCR). This can be calculated by the formula below,[3]

$$ACCR = \frac{DR}{1 - (1 + DR)^{-n}}$$

where, DR is the interest rate, assume 20% in this case and n is the years of compound interest, assume the plant life of 20 years,

$$ACCR = \frac{0.20}{1 - (1 + 0.20)^{-20}} = 0.21$$

$$CAPEX = ACCR \times Total\ installed\ cost$$

$$= 0.21 \times 45{,}514{,}736\ USD = 9{,}558{,}095\ USD/yr$$

The annul capital charge can be added to the operating costs to give a total annualised cost (TAC) with taken the plant operates in 334 days a year,

$$TAC = CAPEX + Operating\ costs$$

$$= 9{,}558{,}095\ \frac{USD}{yr} + (16{,}826 – 73{,}267)\ \frac{USD}{day} \times \frac{334\ day}{1\ yr} = – 9{,}293{,}199\ \frac{USD}{yr}$$

Strategy 2 – Biomass combined heat and power (CHP)

From Table 4, the total MP and HP steam needed is 844,455 kg/day and 48,945 kg/day, respectively. With their heating value as shown in Table A1,

$$Steam\ required{,}D_{steam} = 844{,}455\ kg \times 2.78\,\frac{MJ}{kg} + 48{,}945\ kg \times 3.26\,\frac{MJ}{kg}$$

$$= 2{,}507{,}147\ MJ \times \frac{1.1574 \times 10^{-5}\ MW}{1\ MJ} = 29.02\ MW$$

For Biomass CHP system, the electricity is generated by steam turbines. From Table A2, the power-to-heat ratio of the biomass CHP is 0.13,

$$Power\ produced{,}D_{power} = 29.02\ MW \times 0.13$$

$$= 3.77\ MW \times \frac{1\ MJ}{1.1574 \times 10^{-5}\ MW} = 325{,}929\ MJ$$

Biomass CHP system with the efficiency of 79.6%,

$$Actual\ fuel\ needed\ = (29.02 + 3.77)\ MW \div 0.796 = 41.19\ MW$$

$$Biomasss\ required = 41.19\ MW \times \frac{1\ MJ}{1.1574 \times 10^{-5}\ MW} \div 16.14\,\frac{MJ}{kg} = 220{,}498\ kg\ biomass$$

The biomass utility cost on 0.05 USD/kg biomass Susanto *et al.*,[4]

$$Cost\ of\ biomass\ = 220{,}498\ kg\ biomass \times 0.05\,\frac{USD}{kg\ biomass} = 11{,}025\ USD$$

$$Saving\ cost = \left(325{,}929\ MJ \times 0.028\,\frac{USD}{MJ\ electric}\right) + \left(893{,}400\ kg \times 0.012\,\frac{USD}{kg\ steam}\right)$$

$$= 19{,}847\ USD$$

$$Total\ saving\ cost\ = (19{,}847 - 11{,}025)\ USD\ = 8{,}822\ USD$$

Since the use of renewable sources of biomass, the emissions can be neglected.

$$Total\ reduction\ emissions = Electric\ produce + Steam\ produce$$

$$= \left(325{,}955\ MJ \times 184.8\,\frac{g\ CO_2}{MJ\ electric}\right) + \left(2{,}507{,}147\ MJ \times 75.4\,\frac{g\ CO_2}{MJ\ steam}\right)$$

$$= 249{,}275{,}368\ g\ CO_2 \times \frac{1\ t}{10 \times 10^6\ g} = 249.28\ t\ CO_2$$

The capital cost of biomass CHP system includes the biomass prepare costs, and steam turbine and boiler installed costs. Follow to EPA,[5,6] the preparation cost of biomass and installed cost of steam turbine is 5,430,000 USD and 1,136 USD/kW, respectively. With the required steam turbine capacity of 3.77 MW,

$$Cost\ of\ preparation_{2015}\ =\ 5{,}430{,}000\ USD$$

$$Cost\ of\ preparation_{2023}\ =\ 5{,}430{,}000\ USD \times \left(\frac{789.2}{556.8}\right) = 7{,}696{,}401\ USD$$

$$Cost\ of\ steam\ turbine_{2017} = 3.77\ MW \times \frac{1000\ kW}{1\ MW} \times 1{,}136\ \frac{USD}{kW}$$

$$Cost\ of\ steam\ turbine_{2023} = 4{,}282{,}720\ USD \times \left(\frac{789.2}{567.5}\right) = 5{,}955{,}811\ USD$$

Installed cost of boiler can be calculated by equation below Towler and Sinnott,[7]

$$C_e = a + bS^n$$

Where, $C_e =$ purchased equipment cost
$a,b =$ cost constants
$S =$ size parameter
$n =$ exponent for that type of equipment

Followed to Towler and Sinnott,[7] the boiler a is 124,000, b is 10.0, n is 1 and the required size is 893,400 kg/day with CEPCI index of 532.9,

$$C_{e,boiler} = 124{,}000 + 10(893{,}400 \frac{kg}{day} \times \frac{1\ day}{24\ hr})^1 = 496{,}250\ USD$$

The fixed capital cost is calculated by multiple with the installation factors as shown below Towler and Sinnott,[7]

$$C = \sum_{i=1}^{i=M} C_{e,i,A}[(1 + f_p) + (f_{er} + f_{el} + f_i + f_c + f_s + f_l)/f_m]$$

where, $C_{e,i,A} =$ purchased equipment cost of equipment i in alloy
$M =$ total number of pieces of equipment
$f_p =$ installation factor for piping
$f_{er} =$ installation factor for equipment erection
$f_{el} =$ installation factor for electrical work
$f_i =$ installation factor for instrumentation and process control
$f_c =$ installation factor for civil engineering work
$f_s =$ installation factor for structures and buildings
$f_l =$ installation factor for lagging, insulation, or paint

Taken the factor from Towler and Sinnott (Table 7.5),[7]

$$C_{boiler} = 496{,}250\ USD[(1 + 0.2) + (0.6 + 0.2 + 0.15 + 0.2 + 0.1 + 0.05)/1]$$
$$= 1{,}240{,}625\ USD$$

$$Cost\ of\ boiler_{2023} = 1{,}240{,}625\ USD \times \left(\frac{789.2}{532.9}\right) = 1{,}837{,}308\ USD$$

$$Total\ capital\ cost = Cost\ of\ preparation + Steam\ turbine + Boiler$$
$$= (7{,}696{,}401 + 5{,}955{,}811 + 1{,}837{,}308)\ USD = 15{,}489{,}520\ USD$$

$$CAPEX = 0.21 \times 15{,}489{,}520\ USD = 3{,}252{,}799\ \frac{USD}{yr}$$

$$TAC = 3{,}252{,}799\ \frac{USD}{yr} + (11{,}025\text{–}19{,}847)\ \frac{USD}{day} \times \frac{334\ day}{1\ yr} = 306{,}251\ \frac{USD}{yr}$$

Strategy 3 – Recycled hydrogen

From Table 2, the hydrogen produced by the process is 30,226 kg. A compressor is needed for recycled and poses of CO_2 emissions from the used of power. Followed to Richardson *et al.*[8] typical compressor consumes average of 3 kWh/kg of electricity,

$$Electric\ needed,\ D_{electric} = 30{,}226\ kg \times 3\ \frac{kWh}{kg} = 90{,}678\ kWh$$

$$Electric\ cost = 90{,}678\ kWh \times \frac{3.6\ MJ}{1\ kWh} \times 0.028\ \frac{USD}{MJ\ electric} = 9{,}068\ USD$$

$$Electric\ emission = 90{,}678\ kWh \times \frac{3.6\ MJ}{1\ kWh} \times 184.8\ \frac{g\ CO_2}{MJ} = 60{,}326{,}260\ g\ CO_2$$

$$Reduction\ emissions = 3{,}840{,}516\ MJ \times 81.7\ \frac{g\ CO_2}{MJ\ H_2} = 313{,}770{,}157\ g\ CO_2$$

$$Total\ reduction\ emissions\ = (313{,}770{,}157 - 60{,}326{,}260)\ g\ CO_2 \times \frac{1\ t}{10 \times 10^6\ g}$$

$$= 253.44\ t\ CO_2$$

$$Saving\ cost = (3{,}840{,}516\ MJ \times 0.0034\ \frac{USD}{MJ\ H_2}) = 13{,}058\ USD$$

$$Total\ saving\ cost = (13{,}058 - 9{,}068)\ USD = 3{,}990\ USD$$

With the used of centrifugal compressor, given the purchased cost by Towler and Sinnott[9] with CEPCI of 532.9. Assume compressor is already available in the process plant and take the repurpose pipeline cost as capital cost. Followed to Victoria *et al.*,[9] the cost to repurpose pipelines is expected to be average of 22.5 % of new construction costs,

$$C_{e,boiler} = 580{,}000 + 20{,}000(90{,}678 \frac{kg}{day} \times \frac{1\ day}{24\ hr})^{0.6} = 3{,}381{,}589\ USD$$

$$Capital\ cost = 3{,}381{,}589\ USD \times 0.225 = 760{,}858\ USD$$

$$Capital\ cost_{2023} = 760{,}858\ USD \times \left(\frac{789.2}{532.9}\right) = 1{,}126{,}795\ USD$$

$$CAPEX\ =\ 0.21 \times 1{,}126{,}795\ USD = 236{,}627 \frac{USD}{yr}$$

$$TAC = 236{,}627\ \frac{USD}{yr} + (9{,}068 - 13{,}058) \frac{USD}{day}\ \times \frac{334\ day}{1\ yr} = -\ 1{,}096{,}033\ \frac{USD}{yr}$$

Strategy 4 – Water electrolysis

From Table 2, the total hydrogen required is 126,611 kg. Water electrolysis to produce hydrogen through solar energy to replace fossil-based hydrogen to reduce overall process carbon footprint. Followed to Nasser and Hassan[10] given that every 5.27 kg H_2 requires 800 W of electricity generate by the photovoltaic panel (PV),

$$Electric\ required,\ D_{electric} = 126{,}611\ kg\ H_2 \times \frac{800\ W}{5.27\ kg\ H_2} = 19.2MW$$

$$Saving\ cost = (126{,}611\ kg\ H_2 \times 127.06\frac{MJ}{kg} \times 0.0034\frac{USD}{MJ\ H_2}) = 54{,}696\ USD$$

The water cost is taken as 1.44 USD/kL,[11]

$$Water\ cost = 126{,}611\ kg\ H_2 \times \frac{1000\ g}{1\ kg} \div \frac{0.09\ g\ H_2}{1\ L} \times 1.44\frac{USD}{1000L} = 18{,}232\ USD$$

$$Total\ saving\ cost = (54{,}696–18{,}232)\ USD = 36{,}464\ USD$$

$$Reduction\ emissions = (16{,}087{,}134\ MJ\ H_2 \times 81.7\frac{g\ CO_2}{MJ\ H_2}) \times \frac{1\ t}{10 \times 10^6\ g} = 1{,}314.32\ t\ CO2$$

Followed to Lee *et al.*[12] the emissions from PV plant and electrolyser are 0.057 kg CO_2/kW and 3.23 kg CO_2/kg H_2, respectively.

$$CO_2\ emission = \left(126{,}611\ kg\ H_2 \times 3.12\frac{kg\ CO_2}{kg\ H_2}\right) + \left(19.2MW \times \frac{1000\ kW}{MW} \times 0.057\frac{kg\ CO_2}{kW}\right) \times \frac{1\ t}{1000\ kg}$$
$$= 396.12\ t\ CO_2$$

$$Total\ reduction\ emissions = (1{,}314.32 – 396.12)\ t\ CO_2 = 918.20\ t\ CO_2$$

Following Yates *et al.*[11] the installed cost of electrolyser and PV panels are 784 USD/kW and 818 USD/kW, respectively.

$$Total\ capital\ cost_{2020} = Installed\ cost\ of\ electrolyzer + PV$$
$$= 19.2MW \times 1000 \times (784 + 818)\frac{USD}{kW} = 30{,}758{,}400\ USD$$

$$Total\ capital\ cost_{2023} = 30{,}758{,}400\ USD \times \left(\frac{789.2}{596.2}\right) = 40{,}715{,}413\ USD$$

$$CAPEX\ =\ 0.21 \times 40{,}715{,}413\ USD = 8{,}550{,}237\frac{USD}{yr}$$

$$TAC = 8{,}550{,}237\frac{USD}{yr} + (18{,}232\ –54{,}696)\frac{USD}{day} \times \frac{334\ day}{1\ yr} =– 3{,}628{,}739\frac{USD}{yr}$$

Strategy 5 – Waste heat recovery

From the process, the burned coke is assumed completely proceed to CO_2 have a discharge temperature of 977.65 K with total of 143,038 kg/day and specific heat capacity of 0.849 kJ/kg

K.[13,14,15] The flue gas as hot stream is heat up the water temperature to produce MP steam in a counter-current flow heat exchanger. Water with an inlet temperature of 298.15 K and assume the minimum temperature difference as 10 °C. Given the flue gas outlet temperature of 308.15 K.

$$MP\ steam\ generate, D_{MP\ steam}$$
$$= 143{,}038\ kg \times (977.65 - 308.15)\ K \times 0.849\ \frac{kJ}{kg\ K} \div 1000\ \frac{kJ}{MJ} = 81{,}304\ MJ \div 2.78\ \frac{MJ}{kg}$$
$$= 29{,}246\ kg\ MP\ steam$$

$$Saving\ cost = 29{,}246\ kg \times 0.012\ \frac{USD}{kg\ steam} = 351\ USD$$

$$Reduction\ emissions = 81{,}304\ MJ\ steam \times 75.4\ \frac{g\ CO_2}{MJ\ steam} \times \frac{1\ t}{10 \times 10^6\ g} = 6.13\ t\ CO_2$$

Followed to Towler and Sinnott[7] the purchase cost of heat exchanger can be calculated with a required heat transfer area of 90.29 m^2 calculated by using algebraic approach,

$$Cost\ of\ heat\ exchanger(stainless\ steel) = \left[28{,}000 + 54(90.29)^{1.2}\right]1.3 = 39{,}999\ USD$$

$$Capital\ cost_{2010} = 39{,}999\ USD(1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)$$

$$Capital\ cost_{2023} = 127{,}998\ USD \times \left(\frac{789.2}{532.9}\right) = 189{,}559\ USD$$

$$CAPEX\ =\ 0.21 \times 189{,}559\ USD = 39{,}807\ \frac{USD}{yr}$$

$$TAC = 39{,}807\ \frac{USD}{yr} - 351 \frac{USD}{day} \times \frac{334\ day}{1\ yr} =- 77{,}427\ \frac{USD}{yr}$$

The utility cost used in every reduction strategy is summarised in Table S5 and the parameters of the cogeneration system is shown in Table S6.

Table S5: Utility costs

Utility	Heating Value	Unit	Source
MD-pressure steam	2.78	MJ/kg	Koretsky[16]
HP-pressure steam	3.26	MJ/kg	
Natural gas	47.14	MJ/kg	Abella *et al.*[14]
Hydrogen	127.06	MJ/kg	
Biomass	16.14	MJ/kg	Susanto *et al.*[4]
Water	1.44	USD/kL	Yates *et al.*[11]

Table S6: Cogeneration parameter used

System	Power-to-heat ratio	Efficiency	Source
NG-CHP	1.1	69.0%	Abella *et al.*[14]
Steam turbine	0.13	79.6%	

Case Study 2:

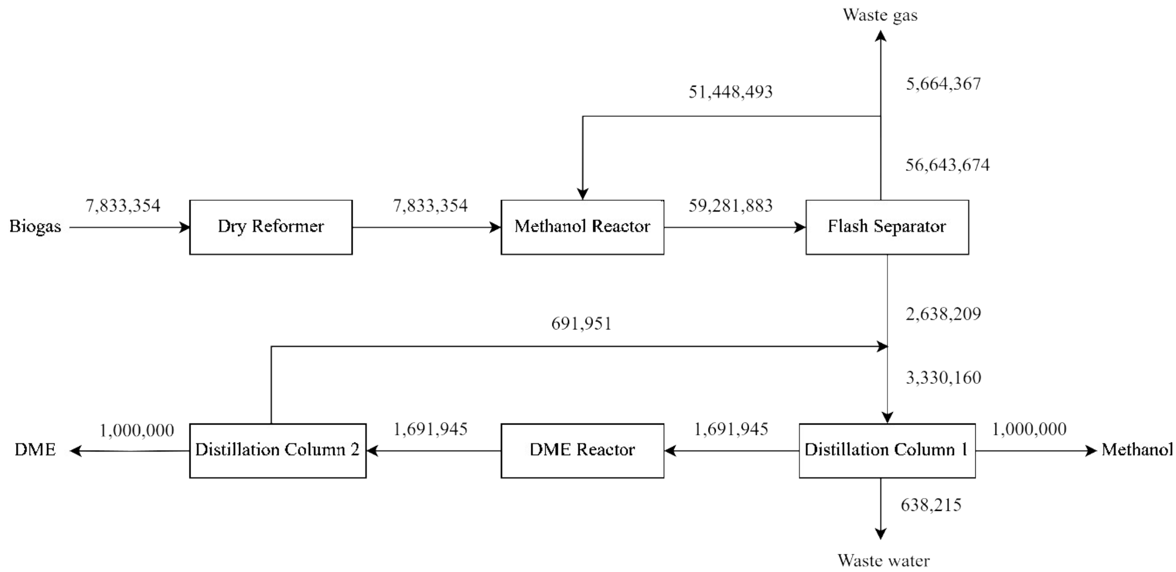

Figure S2: Block diagram of the methanol production case study (numerical values are mass flowrates expressed in kg per day)

Table S7: Methanol process energy flow

Process Energy Process Unit	Power consumption MJ/day	Total Natural Gas requirement kg/day	Medium-pressure steam kg/day	Refrigerant requirement kg/day	Cooling water kg/day
Dry reformer	562,948	752,372	-	-	-
Methanol reactor	47,836,375	-	-	-	16,648,823
Flash separator	-	-	1,031,605	62,191,082	-
Distillation column 1	171	-	9,272,483	671,007	9,587,757
DME reactor	-	57,348	-	-	173,881
Distillation column 2	409,612	-	214,308	-	1,161,134
Total	48,809,106	809,720	10,518,396	62,862,089	27,571,596

Table S8: Methanol process CO_2 emissions

Process CO_2 Emissions Process Unit	Power consumption t CO_{2eq}/day	Total Natural Gas requirement t CO_{2eq}/day	Medium-pressure steam t CO_{2eq}/day	Refrigerant requirement t CO_{2eq}/day	Cooling water t CO_{2eq}/day
Dry reformer	104.03	2,454.30	-	-	-
Methanol reactor	8,840.16	-	-	-	3,299.92
Flash separator	-	-	212.35	382.51	-
Distillation column 1	0.03	-	1,908.67	4.13	1,900.37
DME reactor	-	187.08	-	-	34.46
Distillation column 2	75.70	-	44.11	-	230.15
Total	9,019.92	2,641.38	2,165.13	386.64	5,464.90

Table S9: Methanol process shared and dedicated facilities

Shared facility	Dedicated facility
Dry reformer	
Methanol reactor	DME reactor
Flash separator	Distillation column 2
Distillation column 1	

Case 1 – Heat Integration

Through P-HENS, the optimal heat exchanger network is provided, achieving natural gas and cooling water savings by utilised 3 heat exchangers.

$$Saving\ NG = 13{,}518{,}346.85\ MJ$$

$$Saving\ cooling\ water\ (CW) = 14{,}259{,}175.50\ MJ$$

$$\begin{aligned} Saving\ cost &= Saving\ NG\ \&\ CW \\ &= \left(13{,}518{,}346.85\ MJ \times 0.00265\ \frac{USD}{MJ}\right) + \left(14{,}259{,}175.50\ MJ \times 0.00054\ \frac{USD}{MJ}\right) = 43{,}649.24\ USD \end{aligned}$$

$$\begin{aligned} &Reduction\ emissions \\ &= \left[\left(13{,}518{,}346.85\ MJ \times 69.2\ \frac{g\ CO_2}{MJ\ NG}\right) + \left(14{,}259{,}175.50\ MJ \times 77.73\ \frac{g\ CO_2}{MJ\ CW}\right)\right]\frac{1\ t}{10 \times 10^6\ g} \\ &= 2{,}043.81\ t\ CO_2 \end{aligned}$$

Using an algebraic approach, the required heat transfer areas for the three heat exchangers were calculated as 89,359.77 m^2, 1,607.80 m^2, and 4,861.62 m^2.

$$Cost\ of\ heat\ exchanger(stainless\ steel) = \left[28{,}000 + 54(89{,}359.77\ )^{1.2}\ \right] = 47{,}208{,}680.45\ USD$$

$$Total\ cost\ of\ heat\ exchanger = (47{,}208{,}680.45 + 408{,}076.27 + 1{,}461{,}938.85)\ USD = 49.08\ M\ USD$$

$$Capital\ cost_{2010} = 49.08\ M\ USD(1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)$$

$$Capital\ cost_{2023} = 157.05\ M\ USD \times \left(\frac{789.2}{532.9}\right) = 234.33\ M\ USD$$

$$CAPEX\ = 0.21 \times 234.33\ M\ USD = 49.21\ \frac{M\ USD}{yr}$$

$$TAC = 49.21M\frac{USD}{yr} - 43{,}649.24\ \frac{USD}{day} \times \frac{334\ day}{1\ yr} = 34.63\ \frac{M\ USD}{yr}$$

Case 2 – Compressor ratio

A case study was conducted using Aspen HYSYS, which determined the optimal compressor ratio that utilised the least amount of energy.

$$Saving\ electric = 3{,}372{,}699.29\ MJ$$

$$Saving\ CW = 2{,}780{,}434.90\ MJ$$

$$NG\ requrired = 1{,}412{,}108.06\ MJ$$

$$Saving\ cost = Saving\ electric\ \&\ CW - NG\ required$$
$$= \left(3{,}372{,}699.29\ MJ \times 0.028\,\frac{USD}{MJ}\right) + \left(2{,}780{,}434.90\ MJ \times 0.00054\,\frac{USD}{MJ}\right) - \left(1{,}412\right.$$
$$= 91{,}445.44\ USD$$

$$Reduction\ emissions$$
$$= \left[\left(3{,}372{,}699.29\ MJ \times 184.8\,\frac{g\ CO_2}{MJ}\right) + \left(2{,}780{,}434.90\ MJ \times 77.73\,\frac{g\ CO_2}{MJ\ CW}\right) - \left(1{,}4\right.\right.$$
$$\frac{1\ t}{10 \times 10^6\ g} = 741.68\ \ t\,CO_2$$

To achieve the desired process conditions, four compressors are required, with energy demands of 28,161.05 kW, 28,173.73 kW, 28,213.55 kW, and 28,213.55 kW.

$$Cost\ of\ compressor = \left[580{,}000 + 20{,}000(28{,}161.05)^{0.6}\right] = 9{,}930{,}165.30\ USD$$

$$Total\ cost\ of\ compressor$$
$$= (9{,}930{,}165.30 + 9{,}932{,}691.57 + 9{,}940{,}622.17 + 9{,}940{,}622.17)\ USD = 39.74\ M\ USD$$

$$Capital\ cost_{2010} = 39.74\ M\ USD(1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)$$

$$Capital\ cost_{2023} = 127.18\ M\ USD \times \left(\frac{789.2}{532.9}\right) = 189.76\ M\ USD$$

$$CAPEX\ = 0.21 \times 234.33\ M\ USD = 39.85\,\frac{M\ USD}{yr}$$

$$TAC = 39.85\ M\frac{USD}{yr} - 91{,}445.44\,\frac{USD}{day} \times \frac{334\ day}{1\ yr} = \ 9.31\,\frac{M\ USD}{yr}$$

Case 3 – Recycle ratio

A case study was conducted using Aspen HYSYS, which determined the optimal recycle ratio that utilised the least amount of energy.

$Saving\ electric = 20{,}884{,}050.22\ MJ$

$Saving\ steam = 1{,}858{,}019.61\ MJ$

$Saving\ CW = 4{,}026{,}529.19\ MJ$

$Saving\ refrigerant = 16{,}024{,}943.89\ MJ$

$NG\ requrired = 7{,}136{,}376.45\ MJ$

$$Saving\ cost = \left(20{,}884{,}050.22\ MJ \times 0.028\frac{USD}{MJ}\right) + \left(1{,}858{,}019.61\ MJ \times 0.0044\frac{USD}{MJ}\right) + \left(4{,}02\right.$$
$$+ \left(16{,}024{,}943.89 \times 0.80\frac{USD}{MJ}\right) - \left(7{,}136{,}376.45\ MJ \times 0.00265\frac{USD}{MJ}\right) = 13{,}346{,}27$$

Reducing the recycle ratio requires an additional 1,579,610.75 kg of raw material (biogas).

$$Cost\ of\ biogas = 1{,}579{,}610.75\ kg \times 0.16\frac{USD}{kg} = 258{,}266.36\ USD$$

$$Net\ saving = 13{,}346{,}277.36 - 258{,}266.36\ USD = 13{,}088{,}011.01\ USD$$

$$Reduction\ emissions = \left[\left(20{,}884{,}050.22\ MJ \times 184.8\frac{g\ CO_2}{MJ}\right) + \left(1{,}858{,}019.61\ MJ \times 75.4\frac{g\ CO_2}{MJ}\right) + \left(4{,}02\right.\right.$$
$$\frac{1\ t}{10 \times 10^6\ g} = 4{,}010.26\ t\ CO_2$$

Assume compressor is already available in the process plant and take the repurpose pipeline cost as capital cost. Followed to Victoria *et al.*,[9] the cost to repurpose pipelines is expected to be average of 22.5 % of new construction costs,

$$C_{e,boiler} = 580{,}000 + 20{,}000(128226.10)^{0.6} = 23{,}797{,}521.07\ USD$$

$$Capital\ cost = 3{,}381{,}589\ USD \times 0.225 = 5.35\ M\ USD$$

$$Capital\ cost_{2023} = 5.35\ M\ USD \times \left(\frac{789.2}{532.9}\right) = 7.99\ M\ USD$$

$$CAPEX\ =\ 0.21 \times 7.99\ M\ USD = 1.68\frac{M\ USD}{yr}$$

$$TAC = 1.68\ M\frac{USD}{yr} + 13{,}088{,}011.01\frac{USD}{day} \times \frac{334\ day}{1\ yr} = -\ 4{,}369.72\frac{M\ USD}{yr}$$

Case 4 – Heat integration with recycle ratio

$Saving\ NG = 45{,}111{,}284.15\ MJ$

$Saving\ CW = 16{,}523{,}859.94\ MJ$

$Saving\ refrigerent = 149{,}034.54\ MJ$

$$Saving\ cost = \left(45{,}111{,}284.15\ MJ \times 0.00265\ \frac{USD}{MJ}\right) + \left(16{,}523{,}859.94\ MJ \times 0.00054\ \frac{USD}{MJ}\right) + \left(\right.$$
$$= 254{,}733.60\ USD$$

$$Reduction\ emissions = \left[\left(45{,}111{,}284.15 \times 69.2\ \frac{g\ CO_2}{MJ\ NG}\right) + \left(16{,}523{,}859.94\ MJ \times 77.73\ \frac{g\ CO_2}{MJ\ CW}\right) + \left(149\right.\right.$$
$$\frac{1\ t}{10 \times 10^6\ g} = 4{,}535.80\ t\ CO_2$$

Using an algebraic approach, the required heat transfer areas for the four heat exchangers were calculated as 136,070.11 m^2, 10,010.73 m^2, 2,639.59 m^2, and 168.78 m^2.

$$Cost\ of\ heat\ exchanger(stainless\ steel) = \left[28{,}000 + 54(136{,}070.11)^{1.2}\right] = 78{,}174{,}411.62\ USD$$

$$Total\ cost\ of\ heat\ exchanger = (78{,}174{,}411.62 + 3{,}439{,}555.69 + 717{,}027.98 + 53{,}419.93)\ USD = 82.38\ M\ USD$$

$$Capital\ cost_{2010} = 82.38\ M\ USD(1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)$$

$$Capital\ cost_{2023} = 263.63\ M\ USD \times \left(\frac{789.2}{532.9}\right) = 393.34\ M\ USD$$

$$CAPEX = 0.21 \times 393.34\ M\ USD = 82.60\ \frac{M\ USD}{yr}$$

$$TAC = 82.60M\frac{USD}{yr} - 254{,}733.60\ \frac{USD}{day} \times \frac{334\ day}{1\ yr} = -2.48\ \frac{M\ USD}{yr}$$

Case 5 – Changing compressor ratio with recycle ratio

$$Saving\ electric = 5{,}037{,}977.29\ MJ$$

$$Saving\ CW = 3{,}341{,}114.93\ MJ$$

$$Steam\ requrired = 1{,}696{,}862.36\ MJ$$

$$Saving\ cost = \left(5{,}037{,}977.29\ MJ \times 0.028\ \frac{USD}{MJ}\right) + \left(3{,}341{,}114.93\ MJ \times 0.00054\ \frac{USD}{MJ}\right) - \left(1{,}696\right.$$
$$= 134{,}289.28\ \ USD$$

$$Reduction\ emissions = \left[\left(5{,}037{,}977.29\ MJ \times 184.8\ \frac{g\ CO_2}{MJ}\right) + \left(3{,}341{,}114.93\ MJ \times 77.73\ \frac{g\ CO_2}{MJ\ CW}\right) - \left(1{,}6\right.\right.$$
$$\frac{1\ t}{10 \times 10^6\ g} = \ 1{,}062.77\ \ t\ CO_2$$

To achieve the process conditions, four compressors are required, with energy demands of 33,839.78 kW, 33,855.02 kW, 33,902.88 kW, and 22,500.48 kW.

$$Cost\ of\ compressor = \left[580{,}000 + 20{,}000(33{,}839.78)^{0.6}\ \right] = 11{,}019{,}663.46\ USD$$

$$Total\ cost\ of\ compressor = (11{,}019{,}663.46 + 11{,}022{,}484.10 + 11{,}031{,}338.79 + 8{,}752{,}315.30)\ USD = 41.83\ M\ USD$$

$$Capital\ cost_{2010} = 41.83\ M\ USD(1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)$$

$$Capital\ cost_{2023} = 133.84\ M\ USD \times \left(\frac{789.2}{532.9}\right) = 199.70\ M\ USD$$

$$CAPEX\ = 0.21 \times 199.70\ M\ USD = 41.94\ \frac{M\ USD}{yr}$$

$$TAC = 41.94\ M\frac{USD}{yr} - 134{,}289.28\ \frac{USD}{day}\ \times \frac{334\ day}{1\ yr} =- 2.92\ \frac{M\ USD}{yr}$$

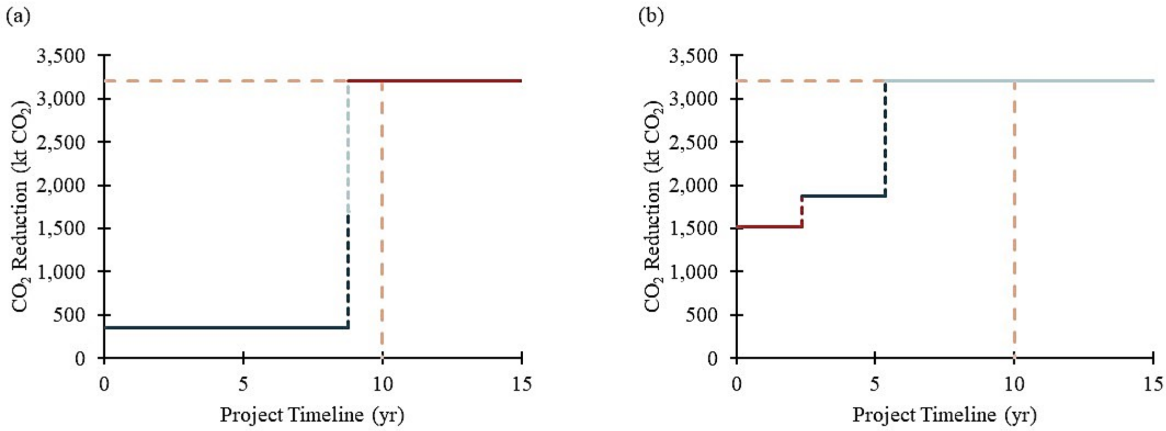

Figure S3: Targeted CO_2 reduction and complete in 10 years in Option 2 a) Result on Figure 17(c), and b) Result on Figure 17(e)

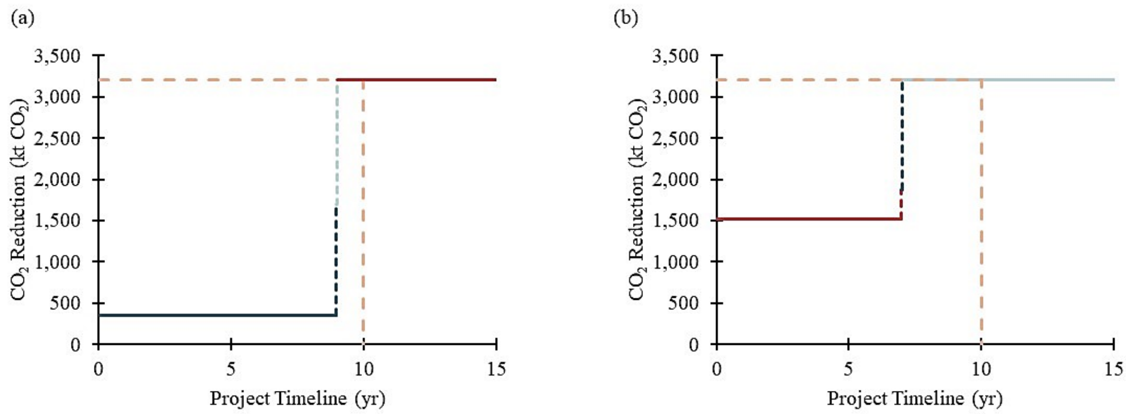

Figure S4: Targeted CO_2 reduction and complete in 10 years on Option 3 a) Result on Figure 18(c), and b) Result on Figure 18(e)

References

1. Epa, Catalog of CHP technologies introduction to CHP technologies, https://nepis.epa.gov/Exe/ZyPDF.cgi/P1010ZR1.PDF?Dockey=P1010ZR1.PDF, (accessed September 2023).
2. Towering Skills, Cost indices, https://toweringskills.com/financial-analysis/cost-indices/, (accessed October 2023).
3. G. Towler and R.A. Sinnott, Principles, practice and economics of plant and process design, Chemical Engineering Design, 2008, 2.
4. H. Susanto, T. Suria and S.H. Pranolo, IOP Publishing, 2018, 334, 1, 012012.
5. EPA, Overview of CHP technologies, https://betterbuildingssolutioncenter.energy.gov/sites/default/files/attachments/Overview_of_CHP_Technologies.pdf, (accessed September 2023).
6. EPA, Catalog of CHP technologies. National Service Center for Environmental Publications (NSCEP), https://www.epa.gov/sites/default/files/2015-07/documents/catalog_of_chp_technologies.pdf, (accessed September 2023).
7. G. Towler and R. Sinnott, Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design, 2013, 5.
8. I.A. Richardson, J.T. Fisher, J.W. Leachman, P.E. Frome, B.O. Smith, S. Guo, S. Chanda, M.S. McFeely and A.M. Miller, Economics Faculty Publications, 2015, 15.
9. PE Media Network, Repurposing pipelines for hydrogen transportation, https://pemedianetwork.com/hydrogen-economist/articles/strategies-trends/2023/repurposing-pipelines-for-hydrogen-transportation/, (accessed November 2023).
10. M. Nasser and H. Hassan, Sustainable Energy Technologies and Assessments, 2023, 60, 103424.
11. J. Yates, R. Daiyan, R. Patterson, R. Egan, R. Amal, A. Ho-Baille and N.L. Chang, Cell Reports Physical Science, 2020, 1, 10.
12. H. Lee, B. Choe, B. Lee, J. Gu, H.S. Cho, W. Won and H. Lim, Journal of Cleaner Production, 2022, 377, 134210.
13. R. Sadeghbeigi, Chapter 1-Fluid catalytic cracking process description—converter section, Fluid Catalytic Cracking Handbook, 2020, 1-22.
14. UCalgary, Petroleum refinery life cycle inventory model (PRELIM) PRELIM v1.4., https://www.ucalgary.ca/sites/default/files/teams/477/prelim-v1.4-documentation.pdf, (accessed August 2023).
15. The Engineering Toolbox, Carbon dioxide – thermophysical properties, https://www.engineeringtoolbox.com/CO2-carbon-dioxide-properties-d_2017.html, (accessed April 2024).
16. M.D. Koretsky, Engineering and chemical thermodynamics, John Wiley & Sons, 2012 Dec 17.