Table 1: Standard enthalpy change and Gibbs energy change for the selected CO_2 reaction pathways.

Reaction	ΔH_R° (kJ/mol)	ΔG_R° (kJ/mol)	Equation
CO_2 (*g*) + $4H_2$ (*g*) → CH_4 (*g*) + $2H_2O$ (*l*)	−253.0	−130.6	(1)
CO_2 (*g*) + $3H_2$ (*g*) → CH_3OH (*l*) + H_2O (*l*)	−131.0	−9.0	(2)
CO_2 (*g*) + H_2 (*g*) → HCOOH (*l*)	−31.2	+33.0	(3)
CO_2 (*g*) + CH_4 (*g*) → 2CO (*g*) + $2H_2$ (*g*)	+247.3	+170.7	(4)

Table 2: Energy auditing using block analysis method for Cases A and B.

Case	Case A			Case B		
Block	I	II+III	IV	I	II+III	IV
Energy Requirement (MW)						
1. Steam requirement for WGS	2.42			2.42		
2. Oxygen production (ASU)	14.83			14.83		
3. Steam requirement in CO_2 capture system (Rectisol)		9.40			9.40	
4. Electricity requirement in CO_2 capture system (Rectisol)		4.98			4.98	
5. CO_2 compressor		2.52				
6. Steam requirement for heating CO_2 feed into methanator					7.63	
7. Air and syngas compressor			9.89			9.89
Sub-total	**17.25**	**16.90**	**9.89**	**17.25**	**22.01**	**9.89**
Energy Generation (MW)						
1. Gasification and syngas cooler	846.77			846.77		
2. Syngas expander	11.75			11.75		
3. CO_2 expander					0.75	
4. Gas turbine			2.64			2.64
5. HRSG			3.31			3.31
6. METHANOL and ACEREACT			49.24			49.24
Sub-total	**858.52**	**0.00**	**55.19**	**858.52**	**0.75**	**55.19**
Net Energy	**841.27**	**−16.90**	**45.30**	**841.27**	**−21.26**	**45.30**

Table 3: Energy auditing using block analysis method for Cases C and D.

Case	Case C			Case D		
Block	I	II+III	IV	I	III	IV
Energy Requirement (MW)						
1. Steam requirement for WGS	16.48			27.50		
2. Oxygen production (ASU)	14.83			14.83	8.96	23.55
3. Steam requirement in CO_2 capture system (Rectisol)		10.44				
4. Electricity requirement in CO_2 capture system (Rectisol)		5.53				
5. CO_2 compressor		7.67				
6. Energy required for tri-reforming process					917.12	
7. Air compressor / syngas compressor			42.88		346.87	9.25
8. Energy for heating feed into GTCOMB.			14.23			24.25
Sub-total	**31.31**	**23.64**	**57.11**	**42.33**	**1272.95**	**57.05**
Energy Generation (MW)						
1. Gasification and syngas cooler	864.61			864.61		
2. Syngas expander	11.56			11.56		
3. Methanol gas expander					60.71	
4. METHANOL					441.00	
5. Gas turbine			85.66			45.4
6. HRSG			105.54			83.1
Sub-total	**876.17**	**0.00**	**191.2**	**876.17**	**501.71**	**128.5**
Net Energy	**844.86**	**−23.64**	**134.09**	**833.84**	**−771.24**	**71.45**

Table 4: Energy auditing using block analysis method for Case E.

Case	Case E	
Block	I	II+III
Energy Requirement (MW)		
1. Oxygen production (ASU)	14.83	
2. Steam requirement for oxidiser		74.23
3. Air compressor		9.78
4. Heat duty for heating Fe_2O_3 (make-up and recycle)		56.37
5. Endothermic heat of reducer		26.01
6. Heat duty for heating Fe_3O_4		44.61
Sub-total	**14.83**	**211.0**
Energy Generation (MW)		
1. Gasification and syngas cooler	846.77	
2. Syngas expander	10.02	
3. CO_2 cooling		141.85
4. H_2 cooling		10.57
5. Exothermic heat of oxidiser		71.23
6. Exothermic heat of combustor		12.61
7. Air cooler		70.41
Sub-total	**856.79**	**306.67**
Net Energy	**841.96**	**95.67**

Table 5: Economic evaluation using block analysis method for Cases A and B.

Case	Case A			Case B		
Block	I	II+III	IV	I	II+III	IV
Capital Cost (million Euro)						
1. GASIFIER	73.4			73.4		
2. WGS	9.2			9.2		
3. SYNGCOOL	33.0			33.0		
4. ASU	40.3			40.3		
5. Expander	3.3			3.3	0.5	
6. Rectisol		61.0			61.0	
7. CO_2 transport and storage		4.5				
8. Compressor		2.4	6.0			6.0
9. Methanator					19.8	
10. Gas turbine			2.2			2.2
11. HRSG			0.5			0.5
12. Methanol reactor			7.3			7.3
13. Acetic acid reactor			14.6			14.6
14. H_2/CO separation			13.2			13.2
Sub-total (million Euro)	**159.2**	**67.9**	**43.7**	**159.2**	**81.3**	**43.7**
Annualised capital cost (million Euro/year)	**17.5**	**7.5**	**4.8**	**17.5**	**8.9**	**4.8**
Operating Cost (million Euro/year)						
1. Coal	53.4			53.4		
2. Hydrogen					164.1	
Sub-total (million Euro/year)	**53.4**	**0.0**	**0.0**	**53.4**	**164.1**	**0.0**
Value of Products (million Euro/year)						
1. Electricity			1.5			1.5
2. Methanol			72.8			72.8
3. Acetic acid			107.0			107.0
4. Hydrogen			20.0			20.0
5. Methane					71.1	
Sub-total (million Euro/year)	**0.0**	**0.0**	**201.3**	**0.0**	**71.1**	**201.3**
Economic Value (million Euro/year) [value of product – (capital cost + operating cost)]	**−70.9**	**−7.5**	**196.5**	**−70.9**	**−101.9**	**196.5**
Total Plant Investment (million Euro/year) [(capital cost + operating cost)]	**70.9**	**7.5**	**4.8**	**70.9**	**173.0**	**4.8**

Table 6: Economic evaluation using block analysis method for Cases C and D.

Case	Case C			Case D		
Block	I	II+III	IV	I	III	IV
Capital Cost (million Euro)						
1. GASIFIER	73.4			73.4		
2. WGS	18.4			9.2		
3. SYNGCOOL	37.1			37.1		
4. ASU	40.3			40.3	31.3	50.8
5. Expander	3.3			3.3	10.1	
6. Rectisol		77.1				
7. CO_2 transport and storage		6.4				
8. Compressor		5.0	16.0		64.8	5.7
9. Tri-reformer					43.4	
10. Gas turbine			29.8			18.5
11. HRSG			15.3			12.0
12. Methanol reactor					31.8	
13. PSA						44.7
Sub-total (million Euro)	**172.5**	**88.5**	**61.1**	**163.3**	**181.4**	**131.7**
Annualised capital cost (million Euro/year)	**19.0**	**9.8**	**6.7**	**18.0**	**20.0**	**14.5**
Operating Cost (million Euro/year)						
1. Coal	53.4			53.4		
2. Natural gas					383.0	46.3
Sub-total (million Euro/year)	**53.4**	**0.0**	**0.0**	**53.4**	**383.0**	**46.3**
Value of Products (million Euro/year)						
1. Electricity			48.2			25.5
2. Methanol					1246.7	
Sub-total (million Euro/year)	**0.0**	**0.0**	**48.2**	**0.0**	**1246.7**	**25.5**
Economic Value (million Euro/year) [value of product – (capital cost + operating cost)]	**−72.4**	**−9.8**	**41.5**	**−71.4**	**843.7**	**−35.3**
Total Plant Investment (million Euro/year) [(capital cost + operating cost)]	**72.4**	**9.8**	**6.7**	**71.4**	**403.0**	**60.8**

Table 7: Economic evaluation using block analysis method for Case E.

Case	Case E	
Block	I	II+III
Capital Cost (million Euro)		
1. GASIFIER	73.4	
2. SYNGCOOL	33.0	
3. ASU	40.3	
4. Expander	3.0	
5. Chemical looping system		70.6
6. CO_2 transport and storage		8.3
7. Compressor		5.9
Sub-total (million Euro)	**149.7**	**84.8**
Annualised capital cost (million Euro/year)	**16.5**	**9.4**
Operating Cost (million Euro/year)		
1. Coal	53.4	
Sub-total (million Euro/year)	**53.4**	**0.0**
Value of Products (million Euro/year)		
1. Hydrogen		91.4
Sub-total (million Euro/year)	**0.0**	**91.4**
Economic Value (million Euro/year) [value of product – (capital cost + operating cost)]	**−69.9**	**82.0**
Total Plant Investment (million Euro/year) [(capital cost + operating cost)]	**69.9**	**9.4**

Table 8: Summary results of ETII, energy and cost evaluations for Cases A to E.

Case	A	B	C	D	E
	Polygeneration with CCS	Polygeneration with methanation	Cogeneration with CCS	Polygeneration with tri-reforming	Chemical Looping
ETII	**0.47**	**11.19**	**0.58**	**8.74**	**0.38**
Block I					
Coal (MW)	648.1	648.1	648.1	648.1	648.1
Net energy from process units (MW)	841.3	841.3	844.9	833.8	842.0
Overall Net Energy (MW/MW coal)	**1.30**	**1.30**	**1.30**	**1.29**	**1.30**
Total Plant Investment (million Euro/year)	70.9	70.9	72.4	71.4	69.9
Total Plant Investment (Euro/MWh coal)	**13.7**	**13.7**	**14.0**	**13.8**	**13.5**
Block II+III+IV					
Syngas LHV (MW)	412.6	412.6	405.7	400.9	424.7
Additional feed LHV (MW)	0.0	619.8	0.0	2802.6	0.0
Product LHV (MW)	330.8	749.1	0.0	2852.8	345.4
Net energy from process units (MW)	28.4	24.0	110.4	−699.8	95.7
Net energy from streams (product – additional feed) (MW)	330.8	129.3	0.0	50.2	345.4
Overall Net Energy (MW/MW syngas)	**0.87**	**0.37**	**0.27**	**−1.62**	**1.04**
Total Plant Investment (million Euro/year)	12.3	177.9	16.5	463.8	9.4
Total Plant Investment (Euro/MWh syngas)	**3.7**	**53.9**	**5.1**	**144.6**	**2.8**

Table B.1: Standard heat of formation and standard Gibbs energy of formation for various components. (Atkins and Paula, 2005)

Component	Standard heat of formation at 298.15 K, ΔH_f° (kJ/mol)	Standard Gibbs energy of formation at 298.15 K, ΔG_f° (kJ/mol)
CO_2 (*g*)	−393.51	−394.36
H_2 (*g*)	0	0
CH_3OH (*l*)	−238.66	−166.27
H_2O (*l*)	−285.83	−237.13
CH_4 (*g*)	−74.81	−50.72
HCOOH (*l*)	−424.72	−361.35
CO (*g*)	−110.53	−137.17

Table C.1: Economic parameters for evaluating capital cost, operating costs and value of products.

Capital cost					
No.	Process unit	Base Cost (million USD)	Scale factor	Base scale	Scale unit
1	Gasifier (GE type) [a]	62.92	0.67	716	MW coal input
2	Water-gas shift reactor [a]	12.24	0.67	1377	MW LHV coal input
3	Rectisol [b, i]	54.1	0.7	9909	kmol CO_2/h
4	CO_2 transport and storage [c]	5.6 Euro/t CO_2			
5	Methanol reactor [b]	7	0.6	87.5	t MeOH/h
6	Acetic acid reactor [d]	2 times of (5)			
7	H_2/CO separation [b, ii]	28	0.7	9600	kmol/h feed
8	Gas turbine [a]	56	0.75	266	MW
9	HRSG [a]	41.2	1	355	MW heat duty
10	SYNGCOOL [a]	25.4	0.6	77	MW heat duty
11	ASU [a]	35.6	0.5	76.6	t O_2/h
12	Compressor [a]	4.83	0.67	10	MW
13	Expander [a]	2.41	0.67	10	MW
14	Tri-reformer/ Methanator [b, iii]	9.4	0.6	1390	kmol/h feed

Operating cost		
No.	Raw material	Cost Estimation
1	Natural Gas [e]	18 Euro/MWh
2	Coal [e]	2.86 Euro/GJ
3	Hydrogen [f]	1104 Euro/t

Market price		
No.	Product	Price
1	Electricity [e]	70.29 Euro/MWh
2	Methanol [g]	305 Euro/t
3	Acetic acid [h]	550 Euro/t
4	Hydrogen [f]	1104 Euro/t
5	Methane [e]	18 Euro/MWh

Note:

[a] Larson et al., 2005. Economic parameters taken from year 2003. Assume 1USD = 0.9 Euro (2003).

[b] Hamelinck and Faaij, 2002. Economic parameters taken from year 2001. Assume 1 USD = 1.1 Euro (2001).

[c] IPCC, 2005. Cost of CO_2 transport: 0-5 USD/t CO_2; Cost of CO_2 storage: 0.6-8.3 USD/t CO_2. Average values of CO_2 transport and storage are taken. Assume 1 USD = 0.8 Euro (2010).

[d] Cost of acetic acid reactor is estimated based on 2 times of the cost of methanol reactor, as suggested by Zhu and Jones, 2009.

[e] DECC, 2010.

[f] Stigel and Ramezan, 2006.

[g] Methanex, 2011. Contract price valid from April to June 2011.

[h] ICIS pricing, 2010.

[i] Cost of Rectisol is assumed to be 2 times of Selexol, as suggested by Denton, 2003.

[ii] Cost of H_2/CO separation unit is estimated based on the cost of PSA.

[iii] Costs of tri-reformer and methanator are assumed to be the same as the cost of steam reformer.

CEPCI

2001= 394.3; 2003=402.0; 2010 (November)=556.8