Supplementary Materials: Comprehensive Exergy Analysis of Three IGCC Power Plant Configurations with CO_2 Capture

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Table S1. Nomenclature used in the manuscript.

Abbreviation	Description	Units
$\dot{E}$	Exergy in thermal heat entering a subsystem (+)	MW
$\hat{e}$	Molar flow exergy	J·mol^{-1}
$\hat{h}$	Molar enthalpy	J·mol^{-1}
$\dot{n}$	Molar flow rate	mol·s^{-1}
p	Pressure	MPa
$\dot{\Phi}_{des}$	Rate of exergy destruction	MW
$\dot{Q}$	Heat leaving a subsystem (+)	MW
$\hat{s}$	Molar entropy	J·mol^{-1}·K^{-1}
$\dot{\sigma}_{irr}$	Rate of entropy production due to irreversible processes	MW·K^{-1}
T_{env}	Temperature of the reference environment	K
$\dot{W}$	Work leaving a subsystem (+)	MW

1. Overall

Table S2 details the inlet and outlet streams from plant, which are the same for all three plants modeled here. The names of these streams are from the NETL Baseline Model AspenPlus files, which are included as Supplemental materials.

Table S2. Inlet and outlet streams of the overall IGCC process. The names are from NETL Baseline Model in AspenPlus.

Inlet			Outlet		
Original Stream Name	Subsystem	New Stream Name	Stream Name	Subsystem	New Stream Name(s)
Coal	Gasifier	S1	Slag	Gasifier	S2
20 (GT)	GT	A2	CO_2-Prod	CO_2	C3
Air1	ASU	A1	S-out	Claus	L12
Water2	Selexol	L6	Stack	Steam	F8
Makeup-w	Steam	L9	Knockout	various	G3, G4, L7, L8, L10
Makeupw	Claus	L11			

The Knockout exiting the plant consists of all of the knockout, waste, and vent streams exiting the overall plant. All three models analyzed here have the same inlet and outlet streams.

2. Modifications

A few modifications were made during the analysis of both plants, but kept constant between the all models. For example, we added pumps and heat exchangers to that the slurry leaving the Claus system was recycled, mixed with makeup water, and split into three streams that became make-up streams elsewhere in the power plant. These make-up streams were (a) the slurry water from the Gasifier subsystem; (b) the sump water from the Gasifier subsystem; and (c) the scrub water from the Scrubber subsystem. The energy associated with heating and compressing these streams to the appropriate temperatures and pressure was fully taken into account in our analysis. Design specs were implemented in the AspenPlus flowsheet to ensure the streams would be as identical as possible in temperature, pressure, and flowrates for consistency between the subsystems and exergy analyses. The stream "TO-SHIFT" is recycled from the Steam cycle and used as the steam for the WGS reaction; a heater was added in the Steam cycle in order to make the two streams have identical temperature and pressure.

In addition, in order to make the process flow diagram more readable, all streams that flow in between subsystems were renamed based on categories listed in Table S3. This naming structure was used to rename the streams in all three models analyzed. All streams that had a flowrate of zero were excluded in the renaming. The following sections provide more detail on the models that could not be included in the paper due to space restrictions.

Table S3. Categories and their respective label for renamed streams.

Category	Label
Air	A
Carbon Dioxide	C
Fuel	F
Gas	G
Liquid	L
Nitrogen	N
Oxygen	O
Solid	S

The air, oxygen and solid streams are identical in all of the models. They are described below in Tables S4–S6, respectively. They give a comprehensive breakdown of the streams that remain the same in all cases. Table S6 includes the components modeled in the coal and slag.

Table S4. Breakdown of air streams for all three models.

Description	A1	A2
	Air Entering ASU	Air Entering as Diluent in GT Subsystem
Temperature (K)	288	288
Pressure (Mpa)	0.101	0.101
Flowrate (kmol·s^{-1})	7.99	30.74
Enthalpy (MW)	−24.21	−93.15
Entropy (kW·K^{-1})	29.30	112.73
Exergy (MW)	0.18	0.71
Composition (mol %)		
CO_2	0.03	0.03
H_2O	1.08	1.08
N_2	77.19	77.19
Ar	0.94	0.94
O_2	20.76	20.76

Table S5. Breakdown of oxygen streams for all three models.

Description	O1	O2
	Oxygen Sent to Gasifier	Oxygen Sent to Claus
Temperature (K)	363.90	505.22
Pressure (Mpa)	6.76	1.00
Flowrate (kmol·s^{-1})	1.62	0.03
Enthalpy (MW)	2.47	0.17
Entropy (kW·K^{-1})	−45.46	−0.04
Exergy (MW)	22.79	0.29
Composition ((mol %))		
N_2	1.88	1.88
Ar	3.22	3.22
O_2	94.90	94.90

Table S6. Breakdown of solid streams for all three models.

Description	S1	S2
	Inlet Coal	Exiting Slag
Temperature (K)	333	489.10
Pressure (Mpa)	7.24	5.5
Flowrate (kg·s^{-1})	62.20	6.61
Enthalpy (MW)	−119.7	-15.0
Entropy (kW·K^{-1})	−139.4	23.0
Exergy (MW)	1747.43	32.99
Composition (wt %)		
C	63.74	12.56
H	4.50	0.13
O	6.89	0.41
N	1.25	0.00
S	2.51	0.00
Cl	0.29	0.00
MC (H_2O)	11.12	0.00
Total Ash	9.70	86.90
SiO_2	3.18	29.92
CaO	1.56	14.69
MgO	0.16	1.54
Al_2O_3	2.58	24.21
Na_2O	0.32	2.99
K_2O	0.10	0.91
FeO	0.00	3.05
Fe_2O_3	1.80	0.11
Fe	0.00	9.48

3. NETL Baseline Model

Table 5 below gives the new name used for streams in the NETL Baseline Model. It describes the subsystem and whether the stream is entering or exiting. The original stream names can be found in the included AspenPlus NETL Baseline Model.

Table S7. Renamed streams in the NETL Baseline Model following the structure presented in Table S1.

Original Stream Name	New Name	Subsystem	Destination
Coal	S1	Gasifier	In
Slurry-w	L1	Gasifier	In
O2X	O1	Gasifier	In
Sump-w	L2	Gasifier	In
rawgas	F1	Gasifier	Out
slag	S2	Gasifier	Out
Rawgas2	F1	Scrubber	In
Scrubwat	L3	Scrubber	In
SG4	F2	Scrubber	Out
Waste (sour1)	L4	Scrubber	Out
SH1	F2	WGS	In
10	G2	WGS	In
SH9	F3	WGS	Out
C1	F3	Cool	In
C4	F4	Cool	Out
Sour 1 (sour 2)	L5	Cool	Out
Coolsynb	F4	Selexol	In
Tailgasb	F5	Selexol	In
N2-Selex	N1	Selexol	In
Water2	L6	Selexol	In
Clnsynb	F6	Selexol	Out
Toclausb	G1	Selexol	Out
Lp-CO2	C1	Selexol	Out

Table S7. *Cont.*

Original Stream Name	New Name	Subsystem	Destination
Mp-CO2	C2	Selexol	Out
Lp1	C1	CO2	In
Mp1	C2	CO2	In
Co2-prod	C3	CO2	Out
Tegwater	L7	CO2	Out
Air1	A1	ASU	In
Knockout	L8	ASU	Out
ASU-vent	G3	ASU	Out
N2Hot2	N2	ASU	Out
To-selex2	N1	ASU	Out
O2HP	O1	ASU	Out
Oxy1	O2	ASU	Out
GT-N2	N2	GTurbine	In
GT1	F6a	GTurbine	In
20	A2	GTurbine	In
GT7	F7	GTurbine	Out
Oxy2	O2	Claus	In
Sour1	L4	Claus	In
Sour2	L5	Claus	In
Acid1	G1	Claus	In
Makeupw	L11	Claus	In
H2	F6b	Claus	In
S-out	L12	Claus	Out
Tail5	F5	Claus	Out
Toslurryw	L1	Claus	Out
Tosump	L2	Claus	Out
Toscrub	L3	Claus	Out
Flue	F7	Steam	In
Makeup-w	L9	Steam	In
Newstack	F8	Steam	Out
To-shift	G2	Steam	Out
Waste	L10	Steam	Out
Ventgas	G4	Steam	Out

Table S6 through Table S12 give a more in-depth description of each of the streams in the NETL Baseline Model. A description, temperature, pressure, flowrate, enthalpy, entropy, exergy, and composition is presented. The enthalpy and entropy values are from the Aspen model and the exergy values are from our calculations.

Table S8. Breakdown of the carbon dioxide streams in the NETL Baseline Model.

Description	C1	C2	C3
	Low Pressure CO_2 Stream Exiting Selexol	Mid-Pressure CO_2 Stream Exiting Selexol	Supercritical CO_2 Product Stream
Temperature (K)	284.4	293.4	322.8
Pressure (Mpa)	0.15	1.1	15.3
Flowrate (kmol·s^{-1})	1.79	1.14	2.93
Enthalpy (MW)	−705.98	−446.62	−1174.01
Entropy (kW·K^{-1})	−3.94	−20.62	−170.35
Exergy (MW)	36.41	30.11	87.4
Composition (mol %)			
CO	0.00	0.05	0.02
CO_2	99.64	99.16	99.63
H_2	0.00	0.54	0.22
H_2O	0.36	0.06	0.05
N_2	0.00	0.11	0.05
Ar	0.00	0.08	0.03

Table S9. Breakdown of fuel streams in the NETL Baseline Model.

Description	F1	F2	F3	F4	F5	F6	F6a	F6b	F7	F8
	Raw Gas Exiting Gasifier	Scrubbed Gas Exiting the Scrubber	Syngas Exiting WGS	Cooled Syngas	Claus Recycle	Cleaned Syngas	Cleaned Syngas Entering GT	Cleaned Syngas Entering Claus	Flue Gas	Stack Gas
Temperature (K)	489.10	484.07	423	312	308	288.03	291.86	291.86	834.21	413.43
Pressure (MPa)	5.5	5.5	5.429	5.429	5.35	5.2	5.2	5.2	0.11	0.11
Flowrate (kmol·s^{-1})	9.46	8.72	10.40	7.78	0.08	5.15	5.14	0.01	38.56	38.56
Enthalpy (MW)	−1507.27	−1329.80	−1912.88	−1247.98	−25.57	−100.52	−100.37	−0.15	−623.03	−1132.1
Entropy (kW·K^{-1})	24.39	16.31	−375.46	−179.88	−2.23	−140.76	−139.60	−0.21	1256.34	411.8
Exergy (MW)	1312.79	1298.90	1231.9	1214.56	4.24	1102.10	1100.42	1.66	292.52	34.2
Composition (mol %)										
CO	26.89	29.19	0.82	1.10	0.02	1.65	1.65	1.65	0.00	0.00
CO_2	7.26	7.87	30.26	40.35	80.97	4.41	4.41	4.41	0.84	0.84
H_2	20.31	22.05	42.11	56.32	0.96	84.90	84.90	84.90	0.00	0.00
H_2O	43.88	39.10	25.28	0.18	0.20	0.01	0.01	0.01	12.20	12.20
N_2	0.61	0.66	0.56	0.75	13.17	7.94	7.94	7.94	75.21	75.21
Ar	0.55	0.60	0.50	0.67	1.34	1.03	1.03	1.03	0.92	0.92
CH_4	0.01	0.01	0.01	0.01	1.37	0.04	0.04	0.04	0.00	0.00
H_2S	0.49	0.52	0.46	0.62	1.97	0.00	0.00	0.00	0.00	0.00
O_2						0.02	0.02	0.02	10.83	10.83

Table S10. Breakdown of gas streams in the NETL Baseline Model.

Description	G1	G2	G3	G4
	Stream Entering Claus for Sulfur Removal	Water Vapor Exiting Steam Cycle to Be Used in WGS	Vent Gas Exiting ASU	Vent Gas Exiting Steam
Temperature (K)	322	597	302.9	406.4
Pressure (MPa)	0.21	6.03	0.11	0.30
Flowrate (kmol·s^{-1})	0.12	1.68	1.01	0.01
Enthalpy (MW)	−23.98	−392.79	−1.06	−1.81
Entropy (kW·K^{-1})	2.68	−95.86	1.67	−0.33
Exergy (MW)	40.88	35.53	0.47	0.09
Composition (mol %)				
CO_2	44.91		0.24	
H_2O	5.77	100		100
N_2	7.71		91.65	
Ar	0.08		0.87	
H_2S	40.99			
O_2	0.54		7.24	

Table S11. Breakdown of liquid streams in the NETL Baseline Model.

Description	L1	L2	L3	L4	L5
	Water Entering Gasifier	Sump Water Used in HX in Gasifier	Scrubber Water	Sour Water Exiting Scrubber	Sour Water Exiting Cool
Temperature (K)	333	373	343	484.07	370.28
Pressure (MPa)	6	6	8.275	5.5	5.429
Flowrate (kmol·s^{-1})	1.42	2.94	2.40	3.15	2.62
Enthalpy (MW)	−403.67	−826.21	−678.67	−856.14	−736.12
Entropy (kW·K^{-1})	−224.99	−438.64	−366.99	−397.40	−384.02
Exergy (MW)	0.33	2.01	0.86	10.64	2.56
Composition (mol %)					
CO				0.02	
CO_2				0.02	0.36
H_2				0.02	0.04
H_2O	100.0	100.0	100.0	99.94	99.58
H_2S					0.02

Table S11. *Cont.*

Description	L6	L7	L8	L9	L10
	Make-Up Water Entering Selexol	**Water Leaving CO_2 Streams**	**Knockout Water Exiting ASU**	**Make-Up Water Entering Condenser in Steam**	**Waste Exiting Steam**
Temperature (K)	322	303	302.9	293	420.82
Pressure (MPa)	0.21	2.1	0.101	0.1	0.45
Flowrate ($kmol \cdot s^{-1}$)	0.01	0.01	0.09	1.80	0.11
Enthalpy (MW)	−2.42	−1.55	−24.78	−516.01	−31.36
Entropy ($kW \cdot K^{-1}$)	−1.32	−0.90	−14.34	−296.17	−15.53
Exergy (MW)	0.00051	0.0002	6.66 × 10–5	0.01	0.17
Composition (mol %)					
H_2O	100.0	100	100.0	100.0	100.0
H_2S					

Description	L11	L12
	Make-Up Water Added to Claus	**Sulfur Product**
Temperature (K)	293	458.71
Pressure (MPa)	0.1	0.176
Flowrate ($kmol \cdot s^{-1}$)	0.93	0.00650
Enthalpy (MW)	−268.14	0.117
Entropy ($kW \cdot K^{-1}$)	−157.30	0.681
Exergy (MW)	0.0052	30.24
Composition (mol %)		
H_2O	100.0	6.61
S_8		93.39

Table S12. Breakdown of nitrogen streams in the NETL Baseline Model.

Description	N1	N2
	Nitrogen Sent to Selexol	**Nitrogen Sent to GT**
Temperature (K)	303	469
Pressure (MPa)	3.17	3.17
Flowrate ($kmol \cdot s^{-1}$)	0.35	4.90
Enthalpy (MW)	−0.03	24.27
Entropy ($kW \cdot K^{-1}$)	−10.05	−74.26
Exergy (MW)	3.24	50.01
Composition (mol %)		
N_2	99.23	99.24
Ar	0.24	0.24
O_2	0.53	0.52

Figure S1 breaks down each subsystem analyzed in the NETL Baseline Model, showing all entering and exiting material, heat and work streams. Included also is the irreversible entropy production, calculated from Aspen values, and the exergy and normalized exergy destruction, from our calculations.

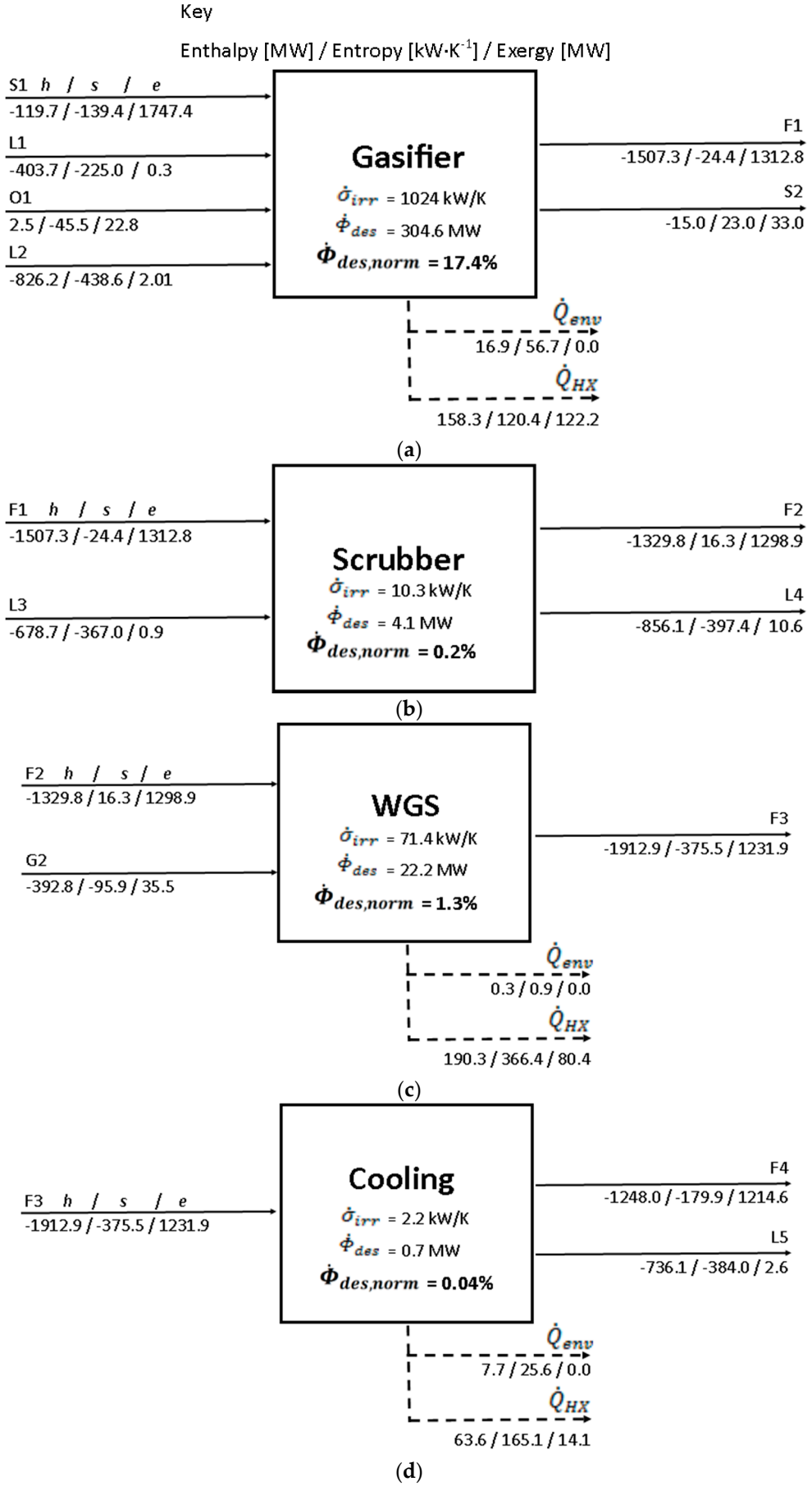
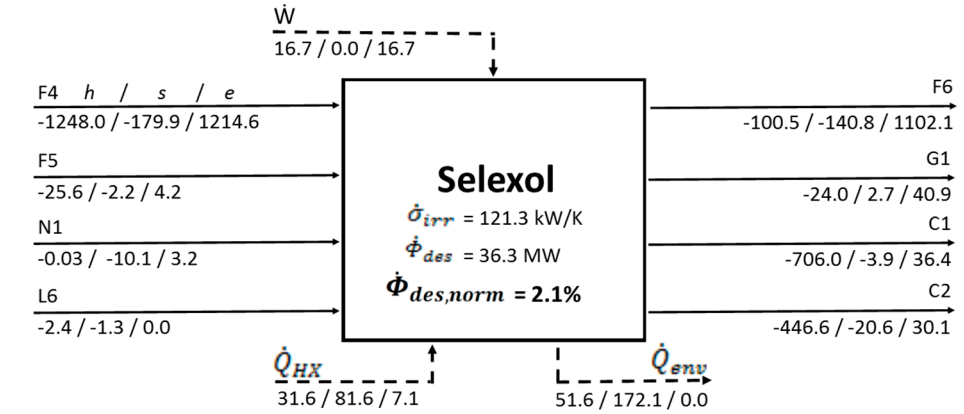


Figure S1. *Cont.*



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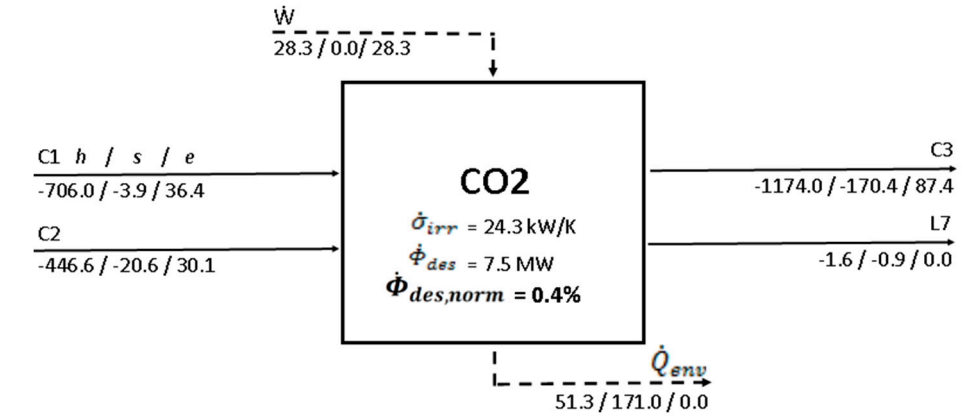

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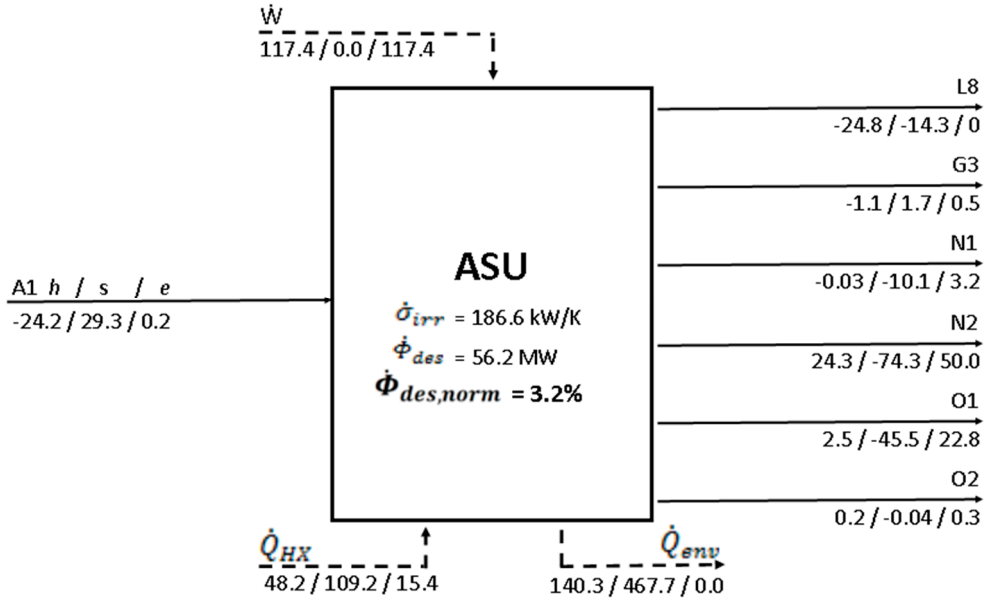

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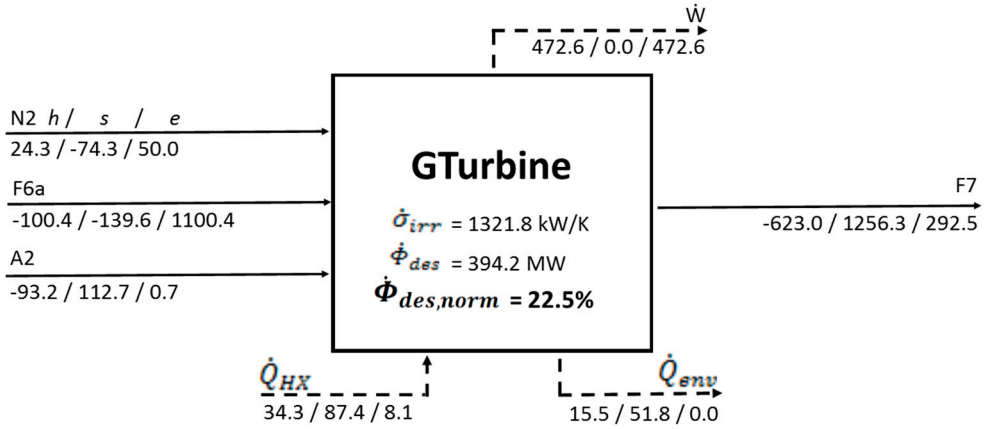
Figure S1. *Cont.*



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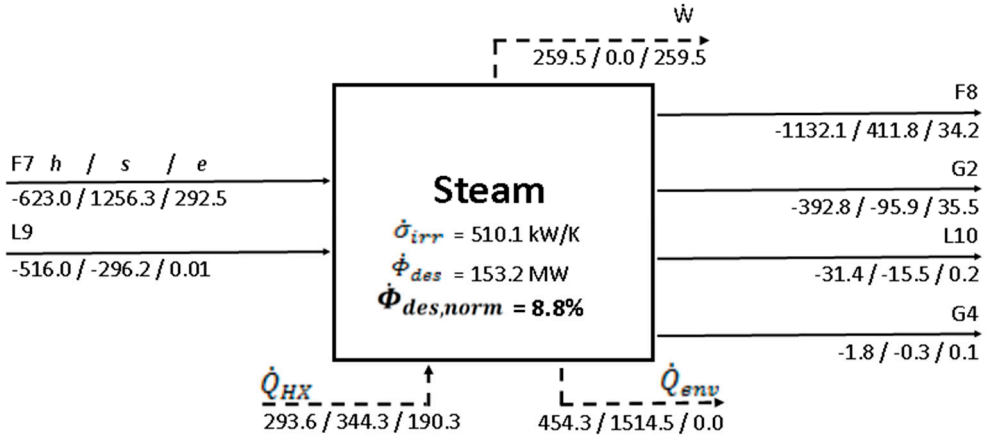

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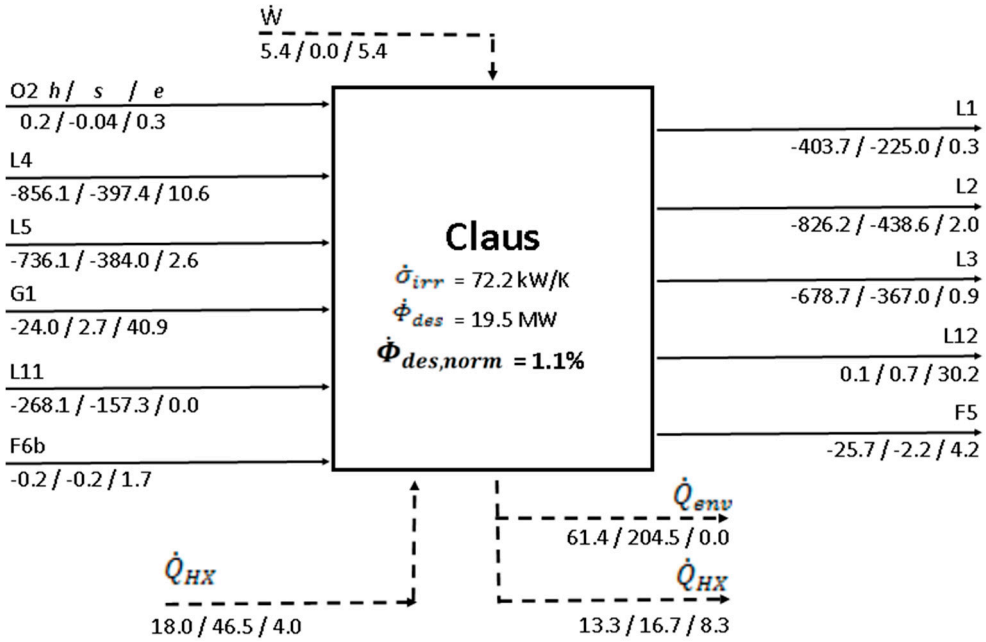

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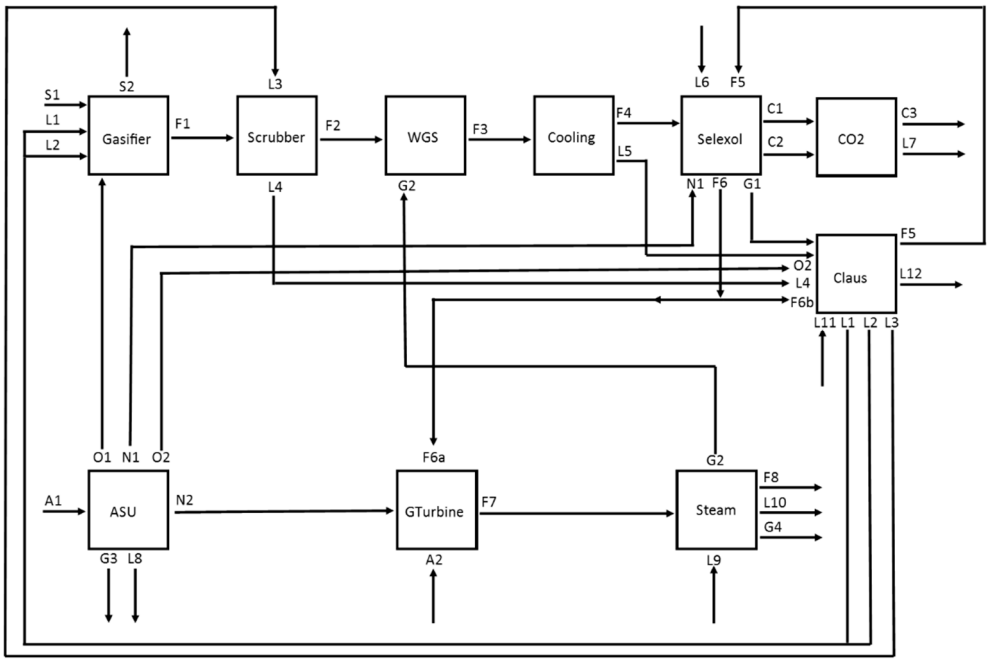
Figure S1. *Cont.*



(**k**)

Figure S1. Breakdown of each subsystem analyzed in the NETL Baseline Model (**a**–**j**). Each diagram includes the enthalpy (MW)/entropy (kW·K^{-1})/exergy (MW) for all material, heat, and work streams, the irreversible entropy production, and the exergy destruction and normalized exergy destruction. (**k**) is the overall process diagram.

4. Hydrogen Membrane Model

The same renaming approach was applied to the Hydrogen Membrane Model, and the new stream names are stated in Table S13.

Table S13. Renamed streams in the Hydrogen Membrane Model following the structure presented in Table S1.

Original Stream Name	New Name	Subsystem	Input/Output
Coal	S1	Gasifier	In
Slurry-w	L1	Gasifier	In
O_2X	O1	Gasifier	In
Sump-w	L2	Gasifier	In
rawgas	F1	Gasifier	Out
slag	S2	Gasifier	Out
Rawgas2	F1	Scrubber	In
Scrubwat	L3	Scrubber	In
SG4	F2	Scrubber	Out
Waste (sour1)	L4	Scrubber	Out
SH1	F2	WGS	In
10	G2	WGS	In
SH9 (23)	F9	WGS	Out
FDHOT (23)	F9	Membrane	In
SWCOLD (24)	N3	Membrane	In
Retcold (26)	F3	Membrane	Out
Percold (25)	F10	Membrane	Out
CO_2 (26)	F3	Cool	In
C4	F4	Cool	Out
Sour 1 (sour 2)	L5	Cool	Out
Coolsynb	F4	Selexol	In
Tailgasb	F5	Selexol	In
N2-Selex	N1	Selexol	In
Water2	L6	Selexol	In
Clnsynb	F6	Selexol	Out
Toclausb	G1	Selexol	Out

Table S13. *Cont.*

Original Stream Name	New Name	Subsystem	Input/Output
Lp-CO_2	C1	Selexol	Out
Mp-CO_2	C2	Selexol	Out
Lp1	C1	CO2	In
Mp1	C2	CO2	In
Co2-prod	C3	CO2	Out
Tegwater	L7	CO2	Out
Air1	A1	ASU	In
Knockout	L8	ASU	Out
ASU-vent	G3	ASU	Out
N2Hot2	N2	ASU	Out
To-selex2	N1	ASU	Out
O_2HP	O1	ASU	Out
Oxy1	O2	ASU	Out
T-Mem2 (24)	N3	ASU	Out
N2Dil	N2	GTurbine	In
GT1	F6a	GTurbine	In
20	A2	GTurbine	In
GT01 (25)	F10	GTurbine	In
GT7	F7	GTurbine	Out
Oxy2	O2	Claus	In
Sour1	L4	Claus	In
Sour2	L5	Claus	In
Acid1	G1	Claus	In
Makeupw	L11	Claus	In
H2	F6b	Claus	In
S-out	L12	Claus	Out
Tail5	F5	Claus	Out
Toslurryw	L1	Claus	Out
Tosump	L2	Claus	Out
Toscrub	L3	Claus	Out
Flue	F7	Steam	In
Makeup-w	L9	Steam	In
Newstack	F8	Steam	Out
To-shift	G2	Steam	Out
Waste	L10	Steam	Out
Ventgas	G4	Steam	Out

Table S14 through Table S18 give a more in-depth description of each of the stream categories. The temperature, pressure, flowrate, enthalpy, entropy, exergy, and composition are presented. The enthalpy and entropy values are from the Aspen model and the exergy values are from our calculations.

Table S14. Breakdown of carbon dioxide streams in the Hydrogen Membrane Model.

Description	C1	C2	C3
	Low Pressure CO_2 Stream Exiting Selexol	Mid-Pressure CO_2 Stream Exiting Selexol	Supercritical CO_2 Product Stream
Temperature (K)	284.42	293.50	322.54
Pressure (MPa)	0.5	1.5	15.3
Flowrate (kmol·s^{-1})	1.60	1.32	2.91
Enthalpy (MW)	−628.83	−519.26	−1170.22
Entropy (kW·K^{-1})	−20.04	−28.03	−170.32
Exergy (MW)	37.21	34.94	86.3
Composition (mol %)			
CO		0.04	0.02
CO_2	99.87	99.53	99.74
H_2	0.01	0.21	0.10
H_2O	0.11	0.05	0.05
N_2		0.09	0.05
Ar	0.01	0.08	0.04

Table S15. Breakdown of fuel streams in the Hydrogen Membrane Model.

Description	F1	F2	F3	F4	F5	F6
	Raw Gas Exiting Gasifier	Scrubbed Gas Exiting the Scrubber	Retentate Entering Cooling	Cooled Syngas	Claus Recycle	Cleaned Syngas
Temperature (K)	489.10	484.07	423	312	308	288.92
Pressure (MPa)	5.5	5.5	5.43	5.43	5.35	5.2
Flowrate (kmol·s^{-1})	9.46	8.72	5.53	5.13	0.07	2.40
Enthalpy (MW)	−1507.27	−1329.80	−1293.40	−1218.70	−23.34	−70.37
Entropy (kW·K^{-1})	−24.39	16.31	−70.05	−113.44	−2.01	−55.66
Exergy (MW)	1312.79	1298.90	579.68	571.64	3.57	457.68
Composition (mol %)						
CO	26.89	29.19	1.50	1.62	0.01	3.45
CO_2	7.26	7.87	55.38	59.65	82.72	6.40
H_2	20.31	22.05	31.68	34.15	0.80	73.03
H_2O	43.88	39.10	7.37	0.20	0.20	0.01
N_2	0.61	0.66	2.27	2.44	11.82	14.87
Ar	0.55	0.60	0.92	0.99	1.48	2.14
CH_4	0.01	0.01	0.02	0.02	1.10	0.07
H_2S	0.49	0.52	0.85	0.92	1.87	
O_2			0.01	0.01		0.03

Description	F6A	F6b	F7	F8	F9	F10
	Cleaned Syngas Entering GT	Cleaned Syngas Entering Claus	Flue Gas	Stack Gas	Syngas Entering the Membrane	Permeate Entering GT
Temperature (K)	293.07	293.07	839.19	405.00	522.51	522
Pressure (MPa)	5.2	5.2	0.105	0.105	5.43	3.16
Flowrate (kmol·s^{-1})	2.39	0.0077	38.56	38.56	10.40	7.65
Enthalpy (MW)	−70.18	−0.19	−1151.64	−1622.94	−1809.36	−518.77
Entropy (kW·K^{-1})	−53.08	−0.15	1208.07	310.06	−147.51	−113.0
Exergy (MW)	456.42	1.25	308.75	40.50	1268.83	698.76
Composition (mol %)						
CO	3.45	3.45			0.82	0.03
CO_2	6.40	6.40	0.87	0.87	30.26	1.10
H_2	73.03	73.03			42.12	34.37
H2O (g)	0.01	0.01	17.97	17.97	25.26	29.02
N_2	14.87	14.87	69.47	69.47	0.56	35.17
Ar	2.14	2.14	0.90	0.90	0.5	0.11
CH_4	0.07	0.07			0.01	
H_2S					0.47	0.02
O_2	0.03	0.03	10.79	10.79		0.18

Table S16. Breakdown of gas streams in the Hydrogen Membrane Model.

Description	G1	G2	G3	G4
	Stream Entering Claus for Sulfur Removal	Water Vapor Exiting Steam Cycle to Be Used in WGS	Vent Gas Exiting ASU	Vent Gas Exiting Steam
Temperature (K)	322	597	301.34	406.38
Pressure (MPa)	0.21	6.03	0.11	0.299
Flowrate (kmol·s^{-1})	0.12	1.68	3.23	0.01
Enthalpy (MW)	−24.33	−392.79	−0.66	−1.65
Entropy (kW·K^{-1})	2.58	−95.86	2.98	−0.30
Exergy (MW)	39.95	35.53	2.12	0.08
Composition (mol %)				
CO_2	46.91		0.07	
H_2O	5.77	100		100
N_2	5.86		96.84	
Ar	0.06		0.48	
H_2S	41.00			
O_2	0.40		2.61	

Table S17. Breakdown of liquid streams in the Hydrogen Membrane Model.

	L1	L2	L3	L4	L5
Description	**Water Entering Gasifier**	**Sump Water Used in HX in Gasifier**	**Scrubber Water**	**Sour Water Exiting Scrubber**	**Sour Water Exiting Cool**
Temperature (K)	333	373	343	484.07	360.42
Pressure (MPa)	6	6	8.275	5.5	5.43
Flowrate (kmol·s^{-1})	1.42	2.94	2.40	3.15	0.40
Enthalpy (MW)	−403.8	−826.6	−682.6	−856.14	−112.6
Entropy (kW·K^{-1})	−224.6	−437.7	−446.9	−397.40	−59.26
Exergy (MW)	0.33	2.01	1.0	10.64	0.38
Composition (mol %)					
CO				0.02	
CO_2				0.02	0.58
H_2				0.02	0.03
H_2O	100.0	100.0	100.0	99.94	99.37
H_2S					0.03

	L6	L7	L8	L9	L10
Description	**Make-Up Water Entering Selexol**	**Water Leaving CO_2 Streams**	**Knockout Water Exiting ASU**	**Make-Up Water Entering Condenser in Steam**	**Waste Exiting Steam**
Temperature (K)	322	303	302.91	293	420.82
Pressure (MPa)	0.21	2.1	0.101	0.10	0.45
Flowrate (kmol·s^{-1})	0.01	0.001	0.09	1.80	0.12
Enthalpy (MW)	−1.46	−0.25	−24.76	−516.20	−31.91
Entropy (kW·K^{-1})	−0.80	−0.15	−14.33	−296.37	−15.80
Exergy (MW)	0.0003	3.25×10^{-5}	6.66×10^{-5}	0.01	1.44
Composition (mol %)					
H_2O	100.0	100.0	100.0	100.0	100.0

	L11	L12
Description	**Make-Up Water Added to Claus**	**Sulfur Product**
Temperature (K)	293	460.02
Pressure (MPa)	0.10	0.18
Flowrate (kmol·s^{-1})	3.61	0.0065
Enthalpy (MW)	−910.00	0.12
Entropy (kW·K^{-1})	−610.02	0.72
Exergy (MW)	0.02	28.53
Composition (mol %)		
H_2O	100.0	6.44
S_8		93.56

Table S18. Breakdown of nitrogen streams in the Hydrogen Membrane Model.

	N1	N2	N3
Description	**Nitrogen Sent to Selexol**	**Nitrogen Sent to GT**	**Nitrogen Sent to Membrane**
Temperature (K)	303	469	364.1
Pressure (MPa)	3.17	3.17	3.17
Flowrate (kmol·s^{-1})	0.23	0.02	2.79
Enthalpy (MW)	−0.02	0.09	4.98
Entropy (kW·K^{-1})	−6.60	−0.28	−63.32
Exergy (MW)	2.13	0.19	25.93
Composition (mol %)			
N_2	99.23	99.24	99.24
Ar	0.24	0.24	0.24
O_2	0.53	0.52	0.52

Figure S2 breaks down each subsystem analyzed in the Hydrogen Membrane Model, showing all entering and exiting material, heat and work streams. Included also is the irreversible entropy production, calculated from Aspen values, and the exergy and normalized exergy destruction, from our calculations.

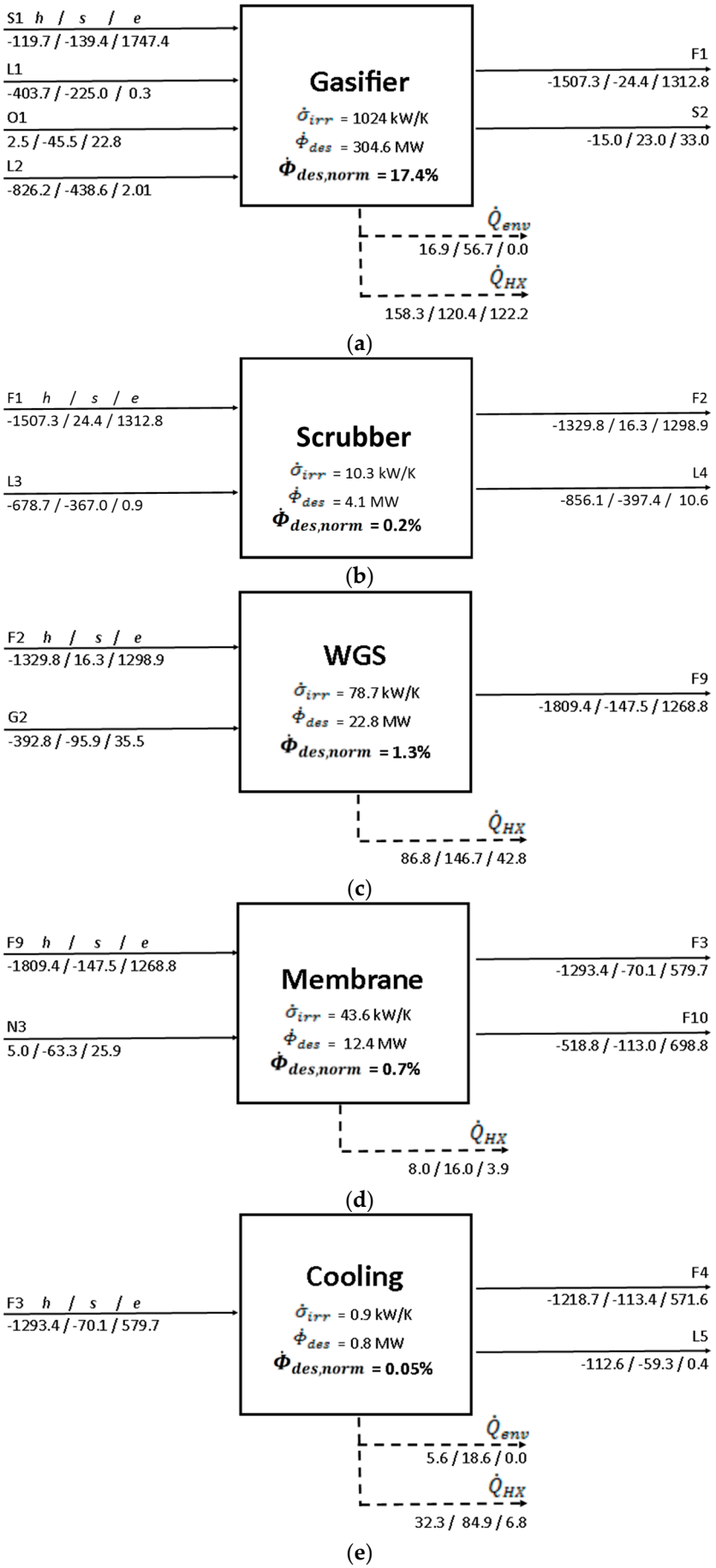
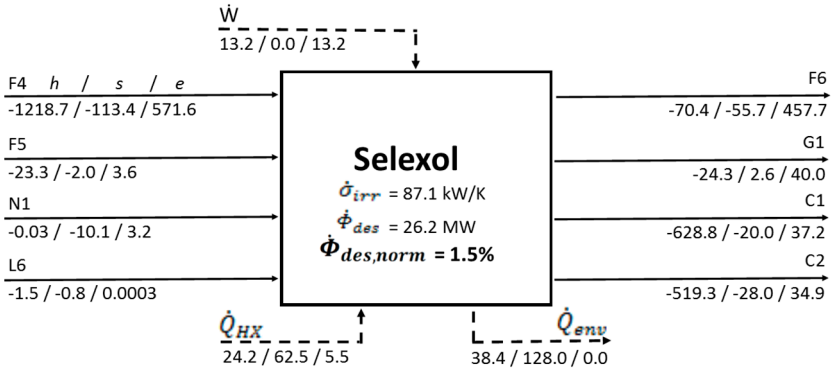


Figure S2. *Cont.*



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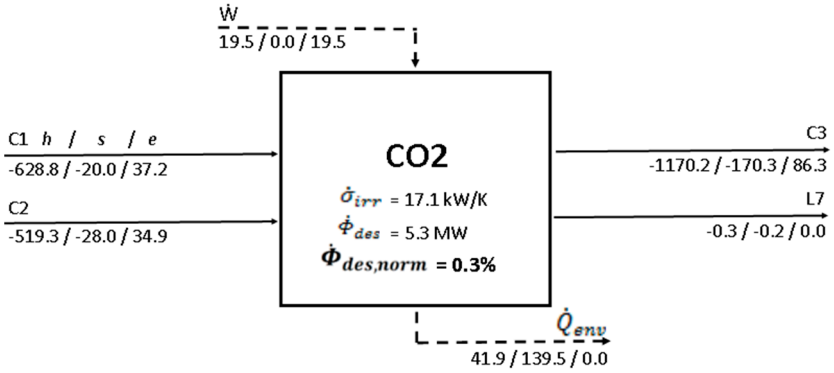

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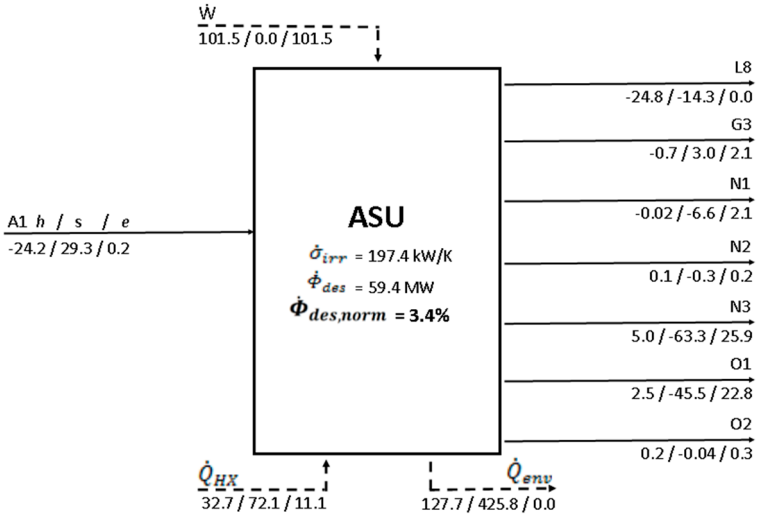

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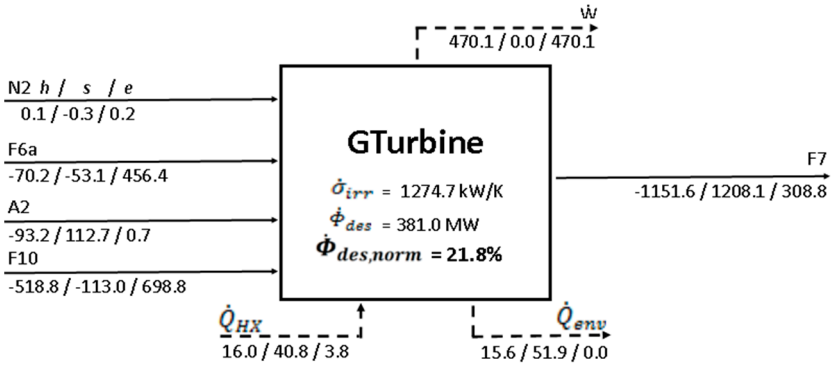

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Figure S2. *Cont.*

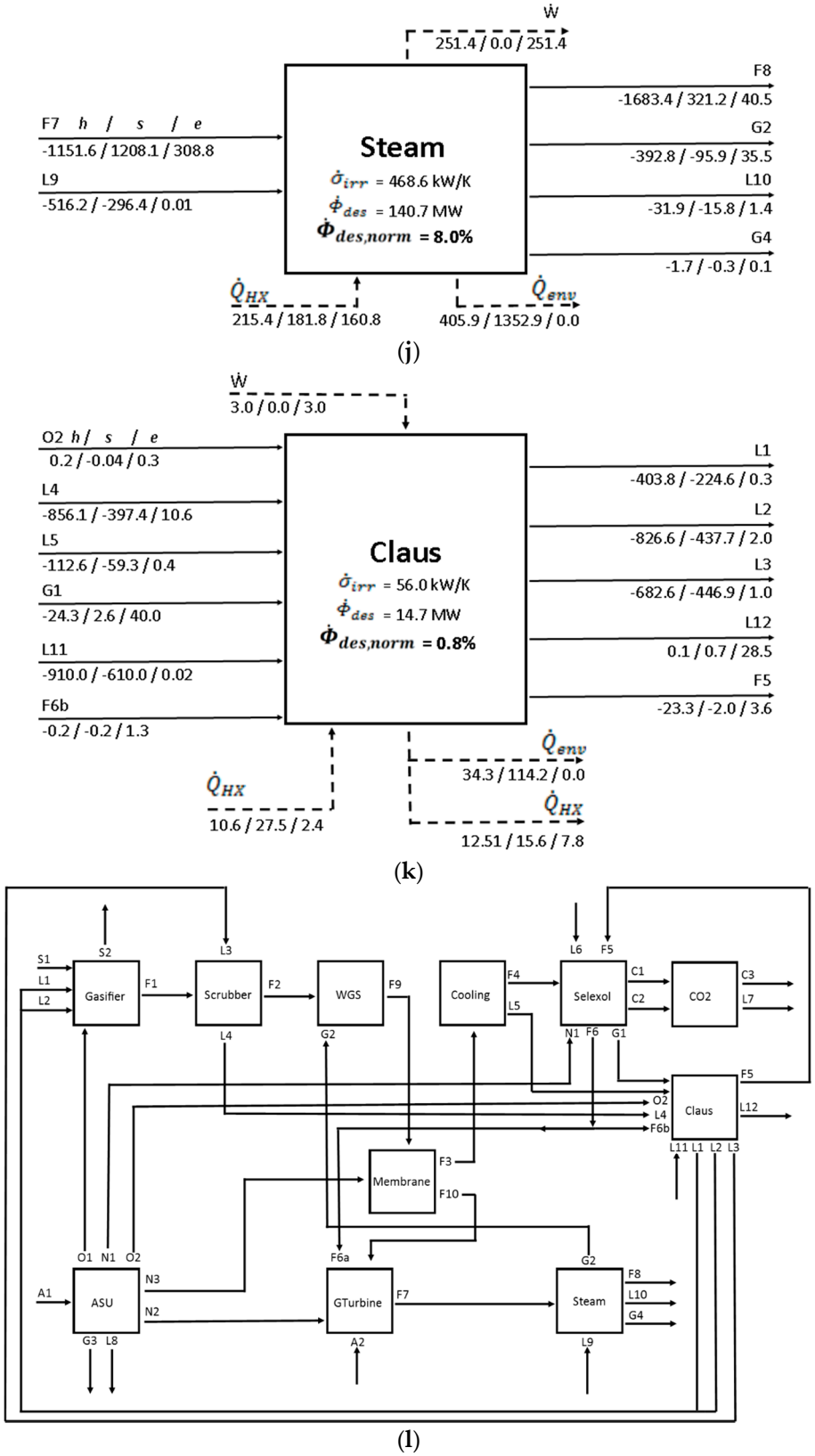


Figure S2. Breakdown of each subsystem analyzed in the Hydrogen Membrane Model (**a**–**k**). Each diagram includes the enthalpy (MW)/entropy (kW·K^{-1})/exergy (MW) for all material, heat, and work streams, the irreversible entropy production, and the exergy destruction and normalized exergy destruction; (**l**) is the overall process flow diagram.

5. CO_2 Membrane Model

Table S19 gives the new names used for streams in the CO_2 Membrane Model. It describes the subsystem and whether the stream is entering or exiting. The original stream names can be found in the included AspenPlus NETL Baseline Model.

Tables 18–22 below gives a more in-depth description of each of the stream categories. A brief description, temperature, pressure, flowrate, enthalpy, entropy, exergy, and composition is presented. The enthalpy and entropy values are from the Aspen model and the exergy values are from our calculations.

Table S19. Renamed streams in the CO_2 Membrane Model following the structure presented in Table S1.

Original Stream Name	New Name	Subsystem	Input/Output
Coal	S1	Gasifier	In
Slurry-w	L1	Gasifier	In
O_2X	O1	Gasifier	In
Sump-w	L2	Gasifier	In
rawgas	F1	Gasifier	Out
slag	S2	Gasifier	Out
Rawgas2	F1	Scrubber	In
Scrubwat	L3	Scrubber	In
SG4	F2	Scrubber	Out
Waste (sour1)	L4	Scrubber	Out
SH1	F2	WGS	In
10	G2	WGS	In
SH9 (23)	F3	WGS	Out
CO_2 (23)	F3	Cool	In
C4	F9	Cool	Out
Sour 1 (sour 2)	L5	Cool	Out
FDHot	F9	Membrane	In
Retcold	F4	Membrane	Out
Percold	C3	Membrane	Out
Coolsynb	F4	Selexol	In
Tailgasb	F5	Selexol	In
NIT2	N1	Selexol	In
Water2	L6	Selexol	In
Clnsynb	F6	Selexol	Out
Toclausb	G1	Selexol	Out
Lp-CO2	C1	Selexol	Out
Mp-CO2	C2	Selexol	Out
Lp1	C1	CO2	In
Mp1	C2	CO2	In
Mem-CO2	C3	CO2	In
Co2-prod	C4	CO2	Out
Tegwater	L7	CO2	Out
Air1	A1	ASU	In
Knockout	L8	ASU	Out
ASU-vent	G3	ASU	Out
N2Hot2	N2	ASU	Out
To-selex2	N1	ASU	Out
O2HP	O1	ASU	Out
Oxy1	O2	ASU	Out
N2Dil	N2	GTurbine	In
GT1	F6a	GTurbine	In
20	A2	GTurbine	In
GT7	F7	GTurbine	Out
Oxy2	O2	Claus	In
Sour1	L4	Claus	In
Sour2	L5	Claus	In
Acid1	G1	Claus	In
Makeupw	L11	Claus	In
H_2	F6b	Claus	In
S-out	L12	Claus	Out

Table S19. *Cont.*

Original Stream Name	New Name	Subsystem	Input/Output
Tail5	F5	Claus	Out
Toslurryw	L1	Claus	Out
Tosump	L2	Claus	Out
Toscrub	L3	Claus	Out
Flue	F7	Steam	In
Makeup-w	L9	Steam	In
Newstack	F8	Steam	Out
To-shift	G2	Steam	Out
Waste	L10	Steam	Out
Ventgas	G4	Steam	Out

Table S20. Breakdown of carbon dioxide streams in the CO_2 Membrane Model.

Description	C1	C2	C3	C4
	Low Pressure CO_2 Stream Exiting Selexol	Mid-Pressure CO_2 Stream Exiting Selexol	CO_2 Permeate from Membrane	Supercritical CO_2 Product Stream
Temperature (K)	284.85	292.93	312	345.45
Pressure (MPa)	0.15	1.1	1.1	15.3
Flowrate (kmol·s^{-1})	0.94	0.10	2.09	3.12
Enthalpy (MW)	−368.64	−36.74	−743.52	−1157.93
Entropy (kW·K^{-1})	−1.85	−1.54	−27.83	−136.63
Exergy (MW)	19.38	4.48	93.67	136.0
Composition (mol %)				
CO	0.02	0.52	0.17	0.14
CO_2	99.38	89.78	90.05	93.20
H_2	0.16	8.15	8.96	6.32
H_2O	0.38	0.07	0.5	0.05
N_2	0.02	0.8	0.12	0.11
Ar	0.04	0.63	0.10	0.11
CH_4		0.04		
H_2S			0.10	**0.07**
O_2		0.01		

Table S21. Breakdown of fuel streams in the CO_2 Membrane Model.

Description	F1	F2	F3	F4	F5	F6
	Raw Gas Exiting Gasifier	Scrubbed Gas Exiting the Scrubber	Syngas Exiting the WGS	Retentate Exiting the Membrane	Claus Recycle	Cleaned Syngas
Temperature (K)	489.10	484.07	423	312	308	288.31
Pressure (MPa)	5.5	5.5	5.43	5.43	5.35	5.2
Flowrate (kmol·s^{-1})	9.46	8.72	10.40	5.68	0.08	4.77
Enthalpy (MW)	−1507.27	−1329.80	−1912.88	−503.95	−26.20	−104.39
Entropy (kW·K^{-1})	−24.39	16.31	−375.46	−136.01	−2.24	−132.70
Exergy (MW)	1312.79	1298.90	1249.85	1116.96	4.36	1053.89
Composition (mol %)						
CO	26.89	29.19	0.82	1.44	0.02	1.7
CO_2	7.26	7.87	30.26	22.08	85.66	5.01
H_2	20.31	22.05	42.11	73.74	1.04	87.72
H_2O	43.88	39.09	25.28	0.07	0.20	0.01
N_2	0.61	0.66	0.56	0.98	8.17	4.46
Ar	0.55	0.60	0.50	0.88	1.30	1.05
CH_4	0.01	0.01	0.01	0.02	1.52	0.04
H_2S	0.49	0.53	0.46	0.81	2.09	
O_2						0.01

Table S21. *Cont.*

Description	F6A	F6b	F7	F8	F9
	Cleaned Syngas Entering GT	Cleaned Syngas Entering Claus	Flue Gas	Stack Gas	Cooled Syngas Entering the Membrane
Temperature (K)	292.18	292.18	834.54	409.15	312
Pressure (MPa)	5.2	5.2	0.10	0.10	5.43
Flowrate (kmol·s^{-1})	4.76	0.01	37.10	37.10	7.78
Enthalpy (MW)	−104.22	−0.17	−603.18	−1110.72	−1247.98
Entropy (kW·K^{-1})	−131.59	−0.22	1215.39	379.26	−179.88
Exergy (MW)	1052.12	1.75	281.58	31.32	1214.57
Composition (mol %)					
CO	1.7	1.7			1.10
CO_2	5.01	5.01	0.89	0.89	40.35
H_2	87.72	87.72			56.32
H_2O (g)	0.01	0.01	12.16	12.16	0.18
N_2	4.46	4.46	74.50	74.50	0.75
Ar	1.05	1.05	0.94	0.94	0.67
CH_4	0.04	0.04			0.01
H_2S					0.62
O_2	0.01	0.01	11.51	11.51	

Table S22. Breakdown of gas streams in the CO_2 Membrane Model.

Description	G1	G2	G3	G4
	Stream Entering Claus for Sulfur Removal	Water Vapor Exiting Steam Cycle to Be Used in WGS	Vent Gas Exiting ASU	Vent Gas Exiting Steam
Temperature (K)	322	597	300.19	406.38
Pressure (MPa)	0.21	6.03	0.11	0.30
Flowrate (kmol·s^{-1})	0.12	1.68	2.37	0.01
Enthalpy (MW)	−24.50	−394.04	−0.81	−1.78
Entropy (kW·K^{-1})	2.51	−97.54	2.56	−0.33
Exergy (MW)	39.31	35.53	1.45	0.09
Composition (mol %)				
CO_2	48.19		0.1	
H_2O	5.77	100		100
N_2	4.68		95.98	
Ar	0.05		0.54	
H_2S	41.00			
O_2	0.31		3.38	

Table S23. Breakdown of liquid streams in the CO_2 Membrane Model.

Description	L1	L2	L3	L4	L5
	Water Entering Gasifier	Sump Water Used in HX in Gasifier	Scrubber Water	Sour Water Exiting Scrubber	Sour Water Exiting Cool
Temperature (K)	333	373	343	484.07	370.28
Pressure (MPa)	6	6	8.275	5.5	5.43
Flowrate (kmol·s^{-1})	1.42	2.94	2.40	3.15	2.62
Enthalpy (MW)	−403.67	−826.6	−682.5	−856.14	−736.12
Entropy (kW·K^{-1})	−224.99	−438.3	−375.4	−397.40	−384.03
Exergy (MW)	0.33	2.01	0.86	10.64	2.56
Composition (mol %)					
CO				0.02	
CO_2				0.02	0.36
H_2				0.02	0.04
H_2O	100.0	100.0	100.0	99.94	99.58
H_2S					0.02

Table S23. *Cont.*

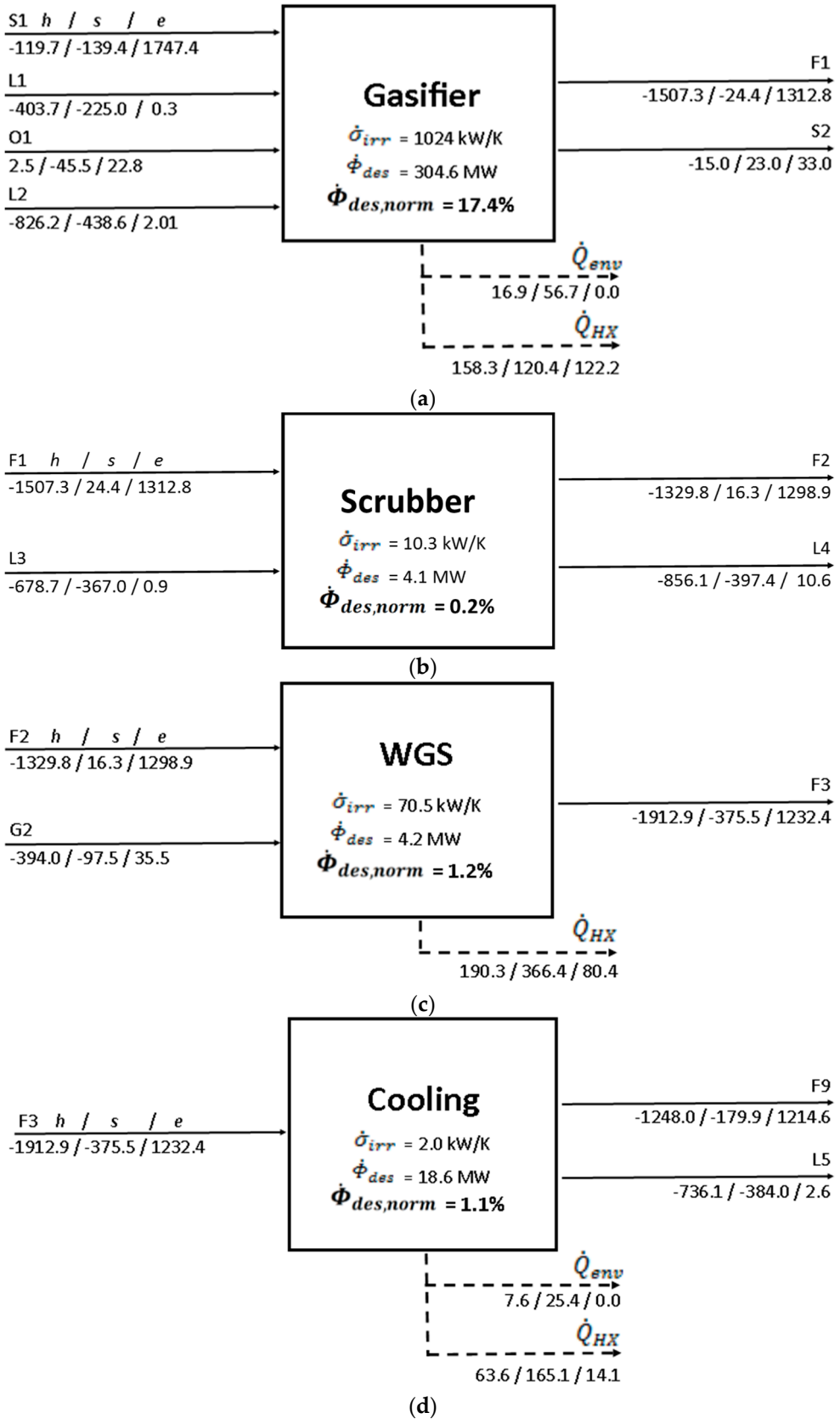
Description	L6	L7	L8	L9	L10
	Make-Up Water Entering Selexol	**Water Leaving Compressed CO_2 Streams**	**Knockout Water Exiting ASU**	**Make-Up Water Entering Condenser in Steam**	**Waste Exiting Steam**
Temperature (K)	322	303	302.91	293	420.82
Pressure (MPa)	0.21	2.1	0.101	0.1	0.45
Flowrate (kmol·s^{-1})	0.002	0.01	0.09	1.80	0.11
Enthalpy (MW)	−0.43	−2.57	−24.77	−515.05	−30.65
Entropy (kW·K^{-1})	−0.24	−2.07	−14.34	−295.71	15.17
Exergy (MW)	9.1×10^{-5}	0.0005	6.66×10^{-5}	0.01	1.38
Composition (mol %)					
H_2O	100.0	100.0	100.0	100.0	100.0

Description	L11	L12
	Make-Up Water Added to Claus	**Sulfur Product**
Temperature (K)	293	458.01
Pressure (MPa)	0.1	0.18
Flowrate (kmol·s^{-1})	0.94	0.00624
Enthalpy (MW)	−271.72	0.11
Entropy (kW·K^{-1})	−159.40	0.70
Exergy (MW)	0.005	28.07
Composition (mol %)		
H_2O	100.0	6.83
S_8		93.17

Table S24. Breakdown of nitrogen streams in the CO_2 Membrane Model.

Description	N1	N2
	Nitrogen Sent to Selexol	**Nitrogen Sent to GT**
Temperature (K)	303	469
Pressure (MPa)	3.17	3.17
Flowrate (kmol·s^{-1})	0.16	3.73
Enthalpy (MW)	−0.01	18.49
Entropy (kW·K^{-1})	−4.49	−56.57
Exergy (MW)	1.45	38.1
Composition (mol %)		
N_2	99.23	99.24
Ar	0.24	0.24
O_2	0.53	0.52

Figure S3 breaks down each subsystem analyzed in the CO_2 Membrane Model, showing all entering and exiting material, heat and work streams. Included also is the irreversible entropy production, calculated from Aspen values, and the exergy and normalized exergy destruction, from our calculations.



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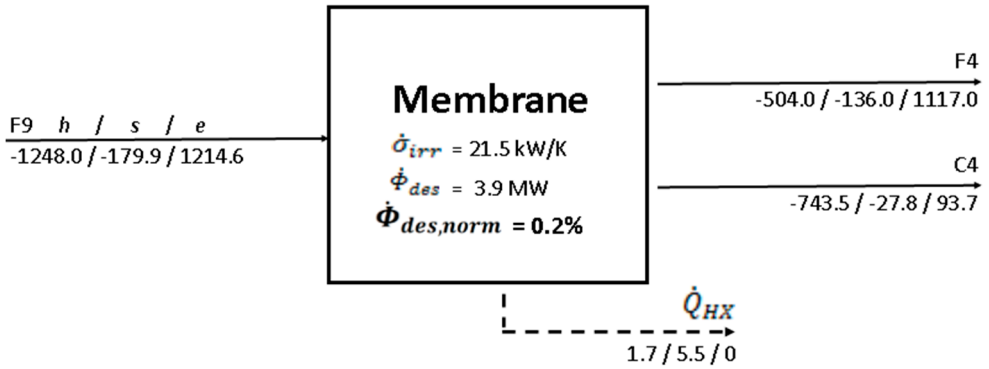

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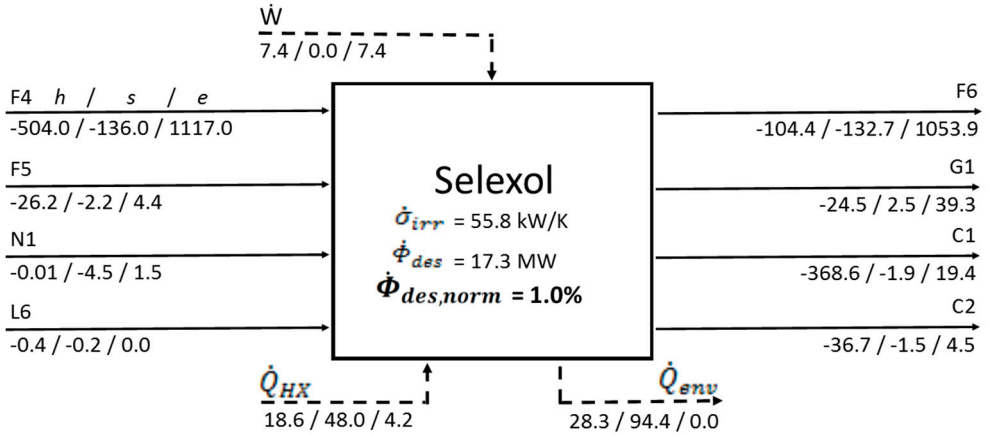

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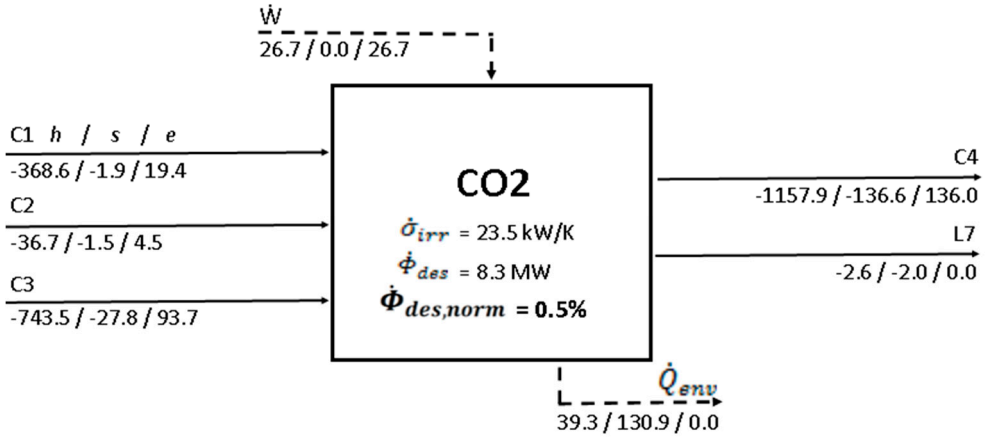

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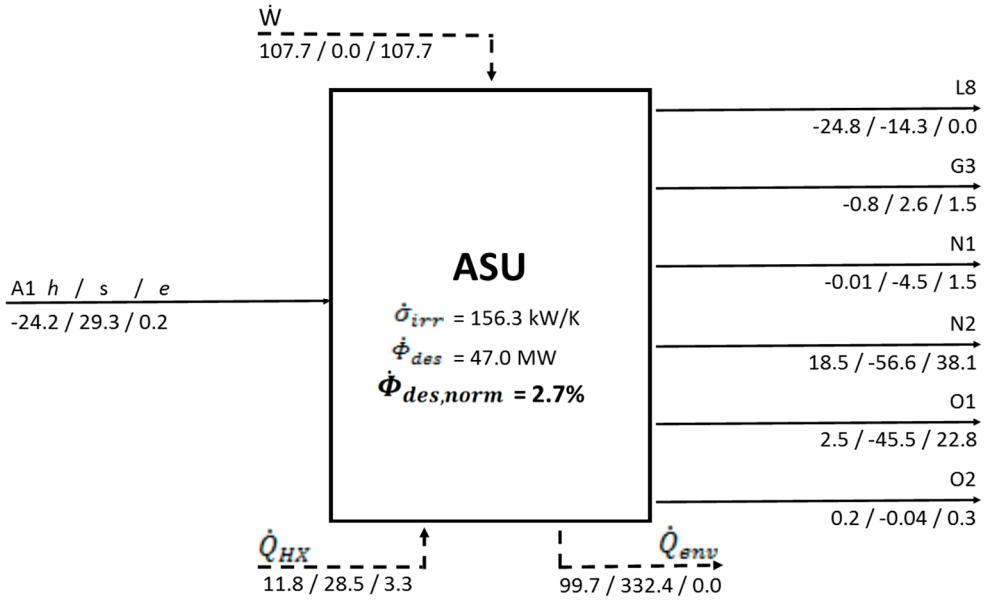

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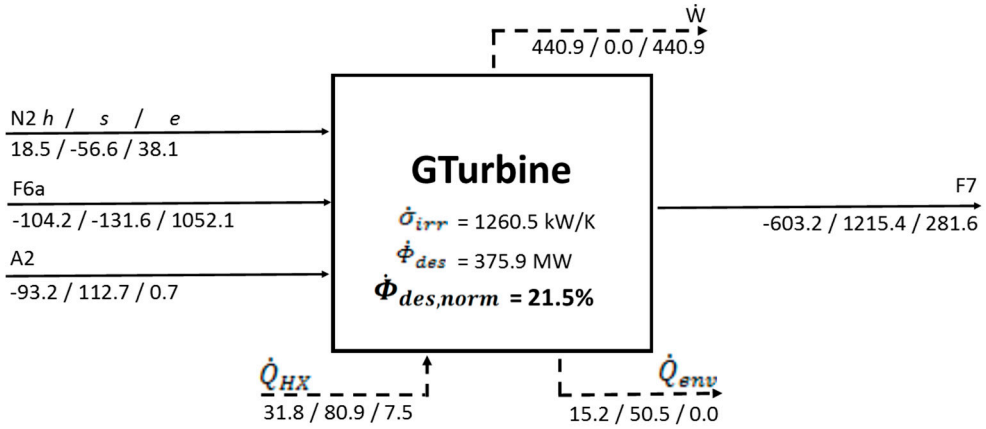

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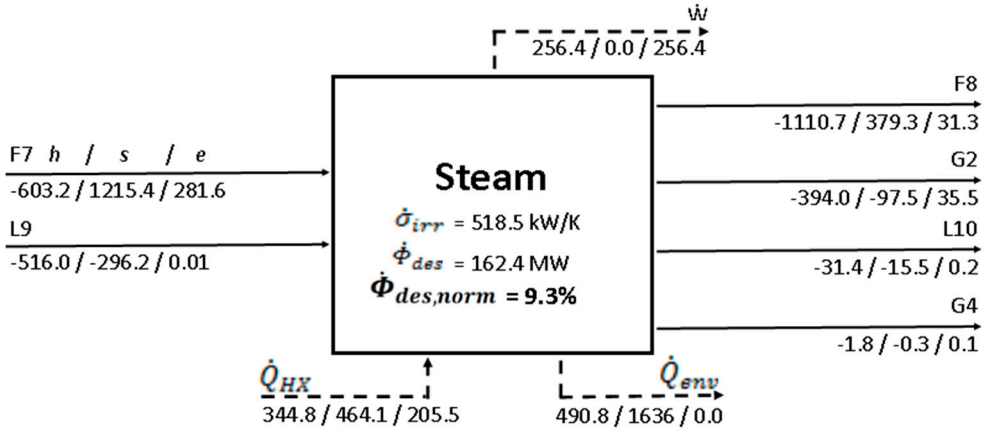

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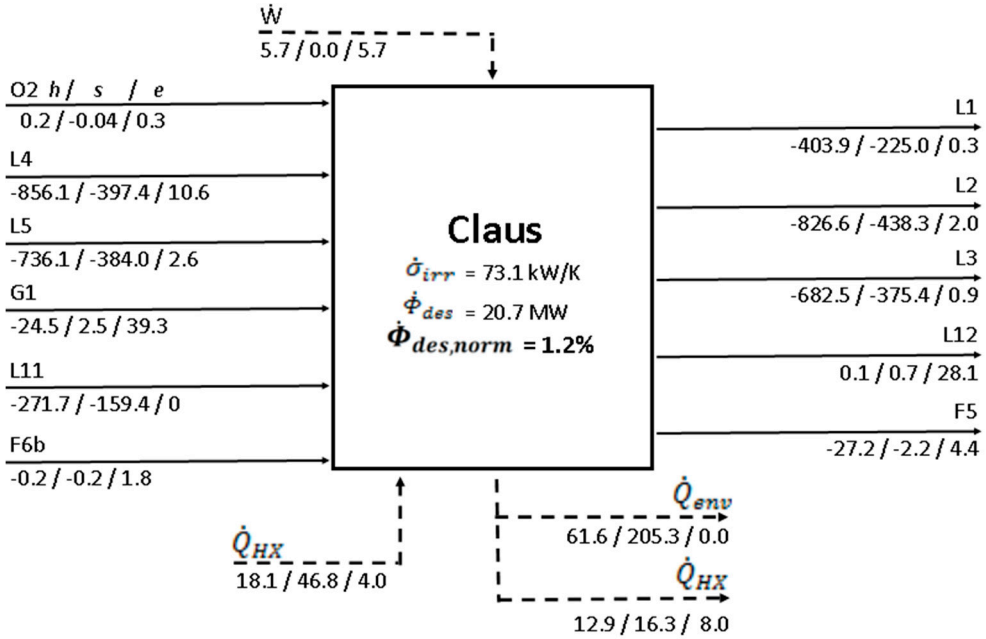
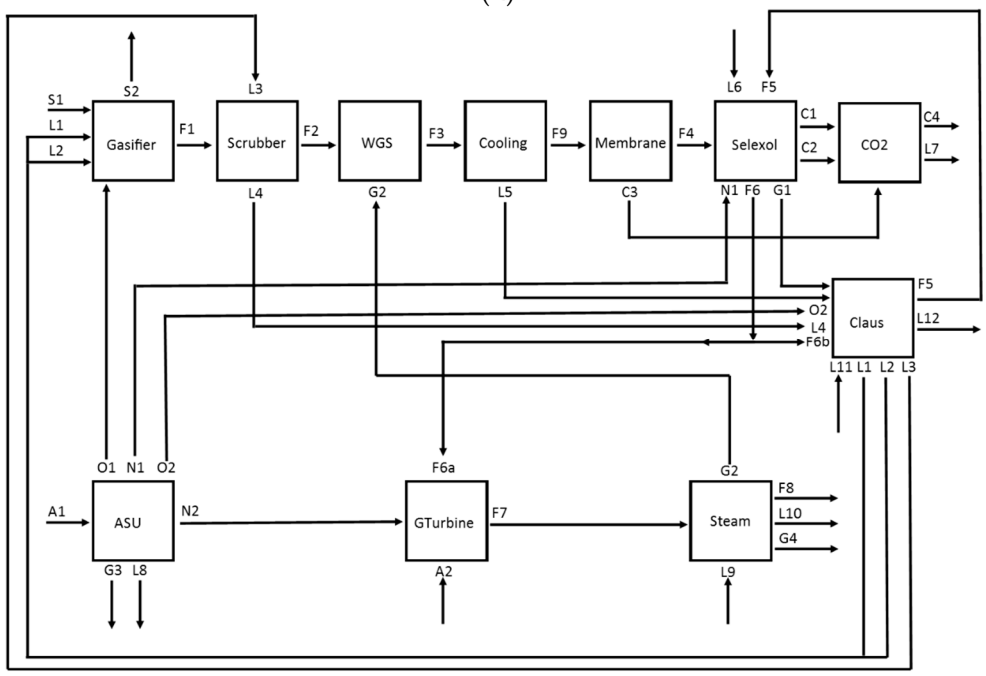


(**k**)



(**l**)

Figure S3. Breakdown of each subsystem analyzed in the CO_2 Membrane Model (**a**–**k**). Each diagram includes the enthalpy (MW)/entropy ($kW \cdot K^{-1}$)/exergy (MW) for all material, heat, and work streams, the irreversible entropy production, and the exergy destruction and normalized exergy destruction; (**l**) is the overall process flow diagram.