



*Driving Innovation ♦ Delivering Results*



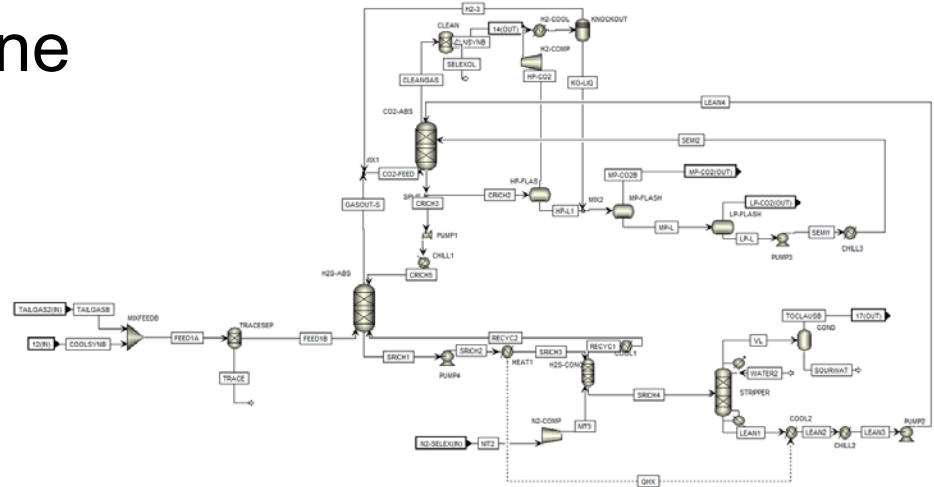
## Comprehensive Exergy Analysis of Three IGCC Power Plant Configurations with CO<sub>2</sub> Capture

Nicholas S. Siefert, Sarah Narburgh, Yang Chen  
August 8, 2016



- IGCC-CCS Overview
- Intro to Exergy Analysis for State-Steady Processes
- Overview of All 3 Cases
  - Baseline Selexol™ Model
  - H<sub>2</sub>-selective membrane
  - CO<sub>2</sub>-selective membrane
- Comparison of Cases
- Conclusions & Future Work

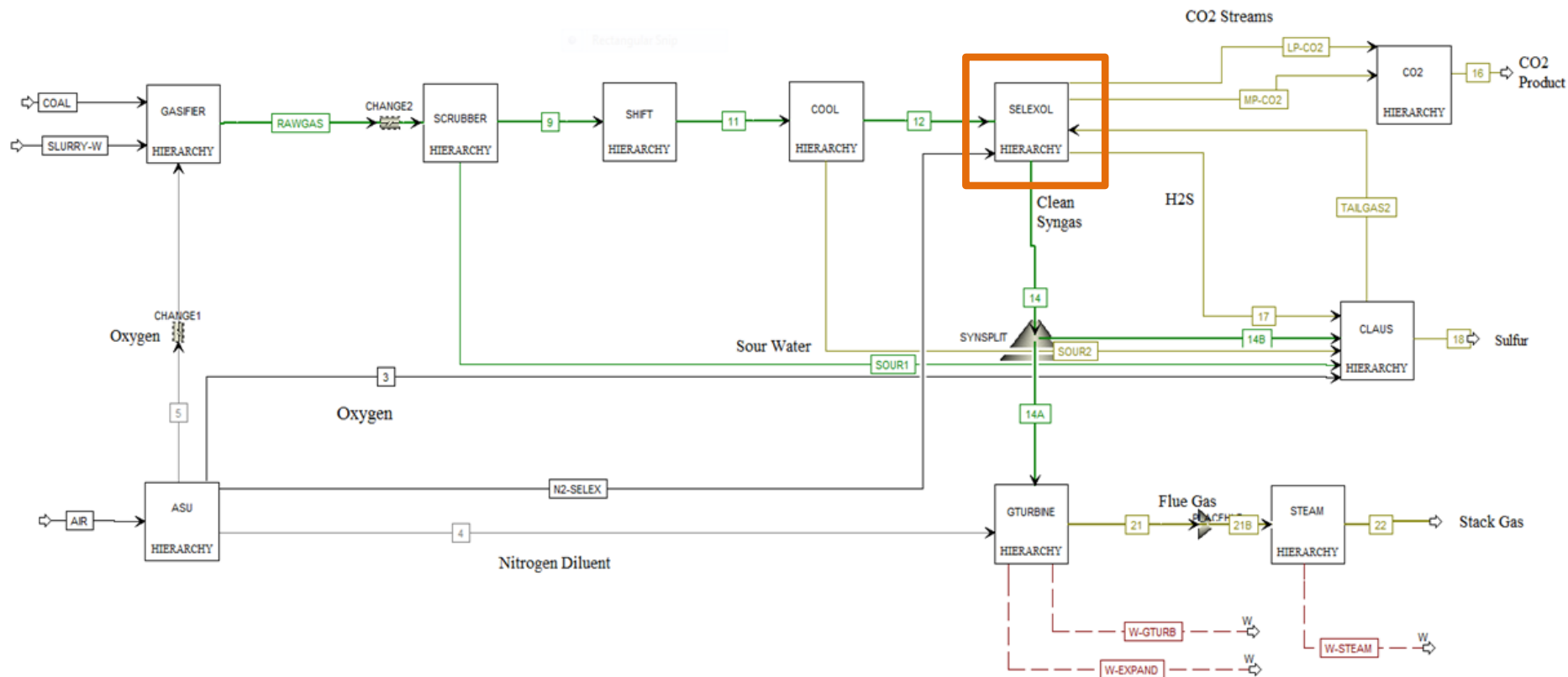
Integrated Gasification Combined Cycle (IGCC)



# Baseline Model includes Ten Subsystems



## GE IGCC with CO2 Capture



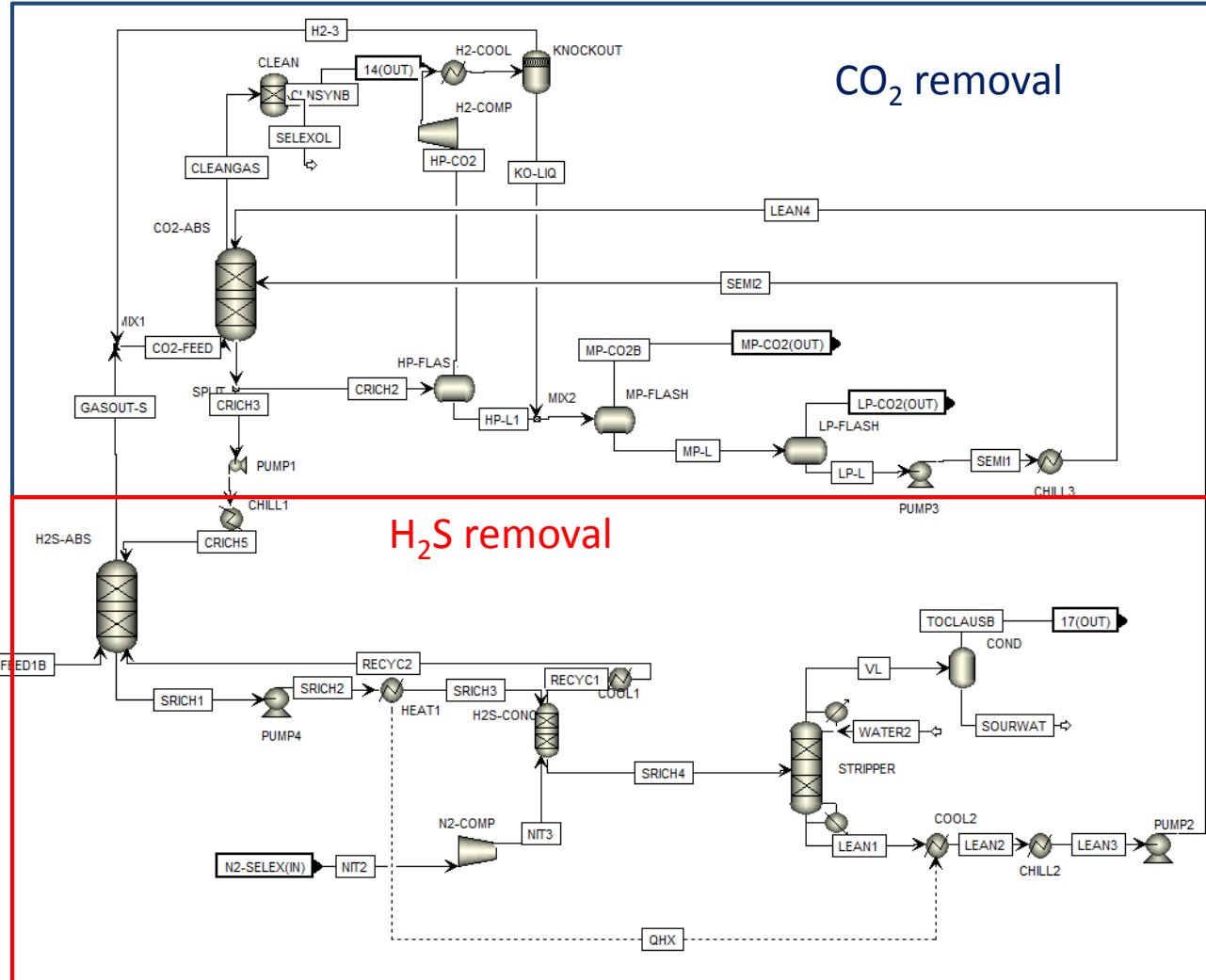
Model #1: Baseline Model from Field and Brasington (2011)  
Based off of NETL's Bituminous Baseline Rev 2 (Nov 2010): GEE IGCC-CCS

# Example Subsystem



2-Stage Selexol subsystem flow sheet

Syngas at 5.4 MPa, 40°C



# Subsystem Analysis: Route#1



Guoy-Stodola Theorem

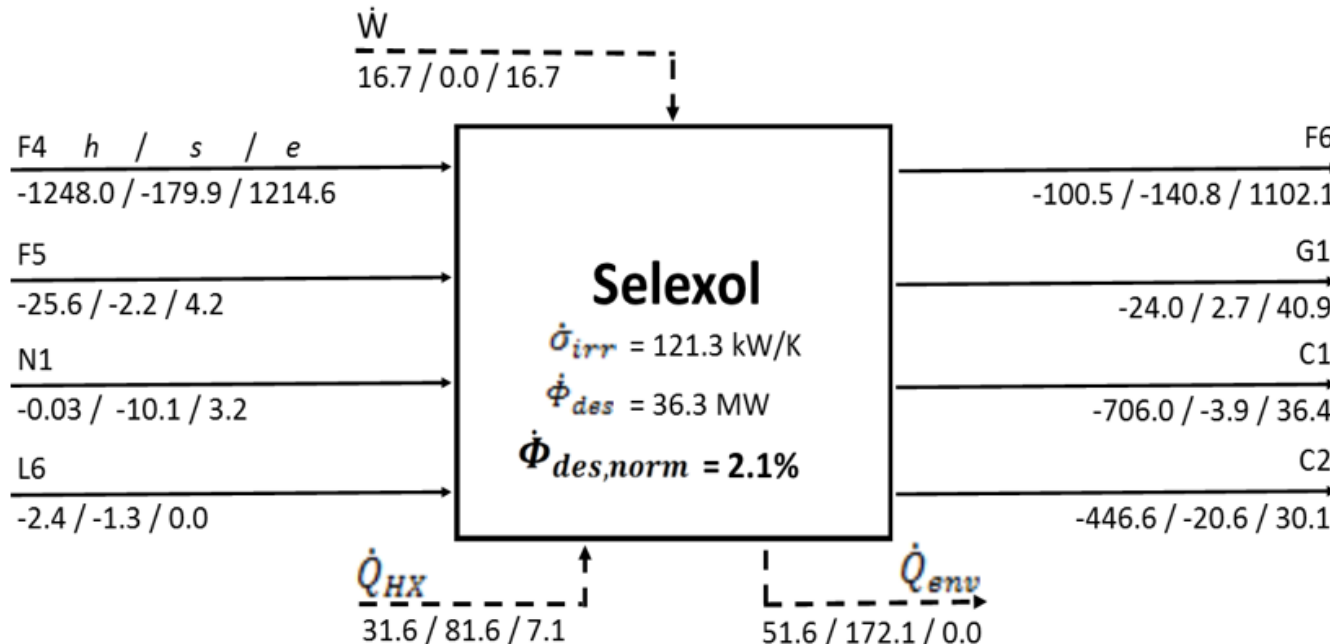
$$\dot{\Phi}_{des} = T_{env} \cdot \dot{\sigma}_{irr}$$

2<sup>nd</sup> Law

$$\dot{\sigma}_{irr} = \frac{\dot{Q}_{env}}{T_{env}} + \sum_{o=outlet} \dot{n}_o \hat{s}_o - \sum_{i=inlet} \dot{n}_i \hat{s}_i + \sum_j \frac{\dot{Q}_j}{T_{j,o} - T_{j,i}} \ln \left( \frac{T_{j,o}}{T_{j,i}} \right)$$

1<sup>st</sup> Law

$$\dot{Q}_{env} = \sum_{i=inlet} \dot{n}_i \hat{h}_i - \sum_{o=outlet} \dot{n}_o \hat{h}_o - \dot{W} - \sum \dot{Q}_j$$



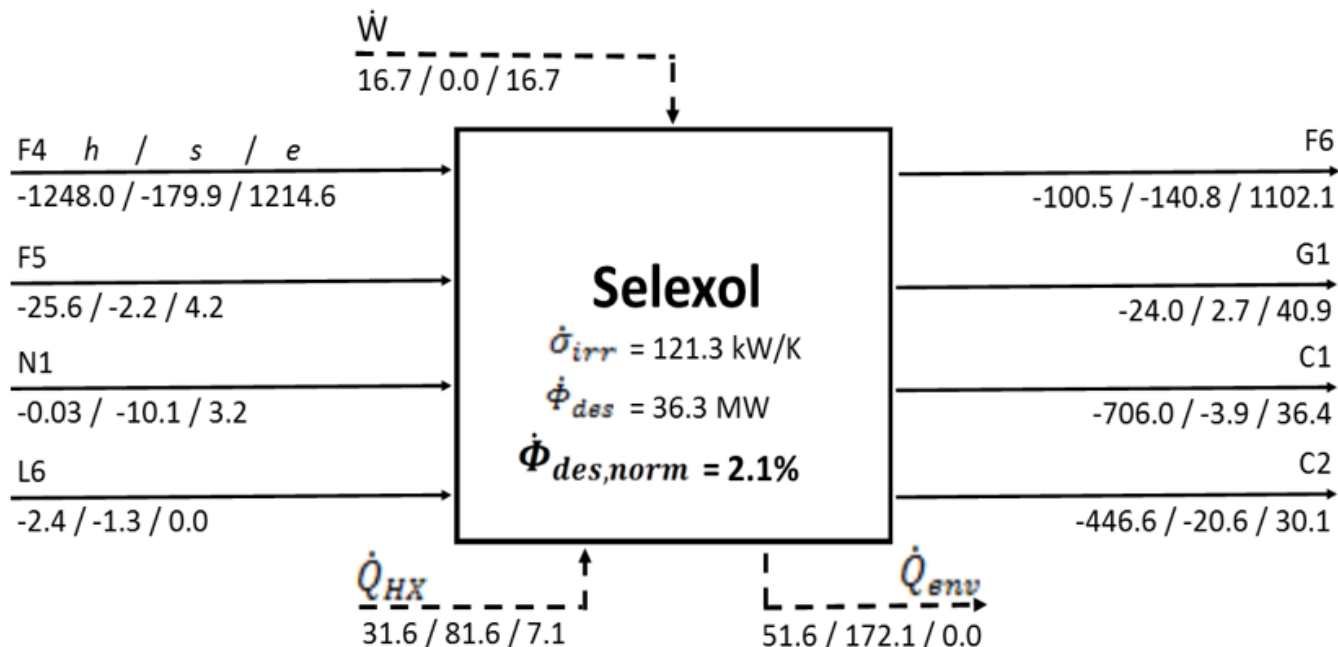
# Subsystem Analysis: Route#2



Exergy Analysis 
$$\dot{\Phi}_{des} = \sum_{i=inlet} \dot{n}_i \hat{e}_i - \sum_{o=outlet} \dot{n}_o \hat{e}_o - \dot{W} - \sum_j \dot{E}_j$$

Exergy of a stream 
$$\hat{e} = [(\hat{h} - \hat{h}_{stp}) - T_{env}(\hat{s} - \hat{s}_{stp})] + \hat{e}_{chem}$$

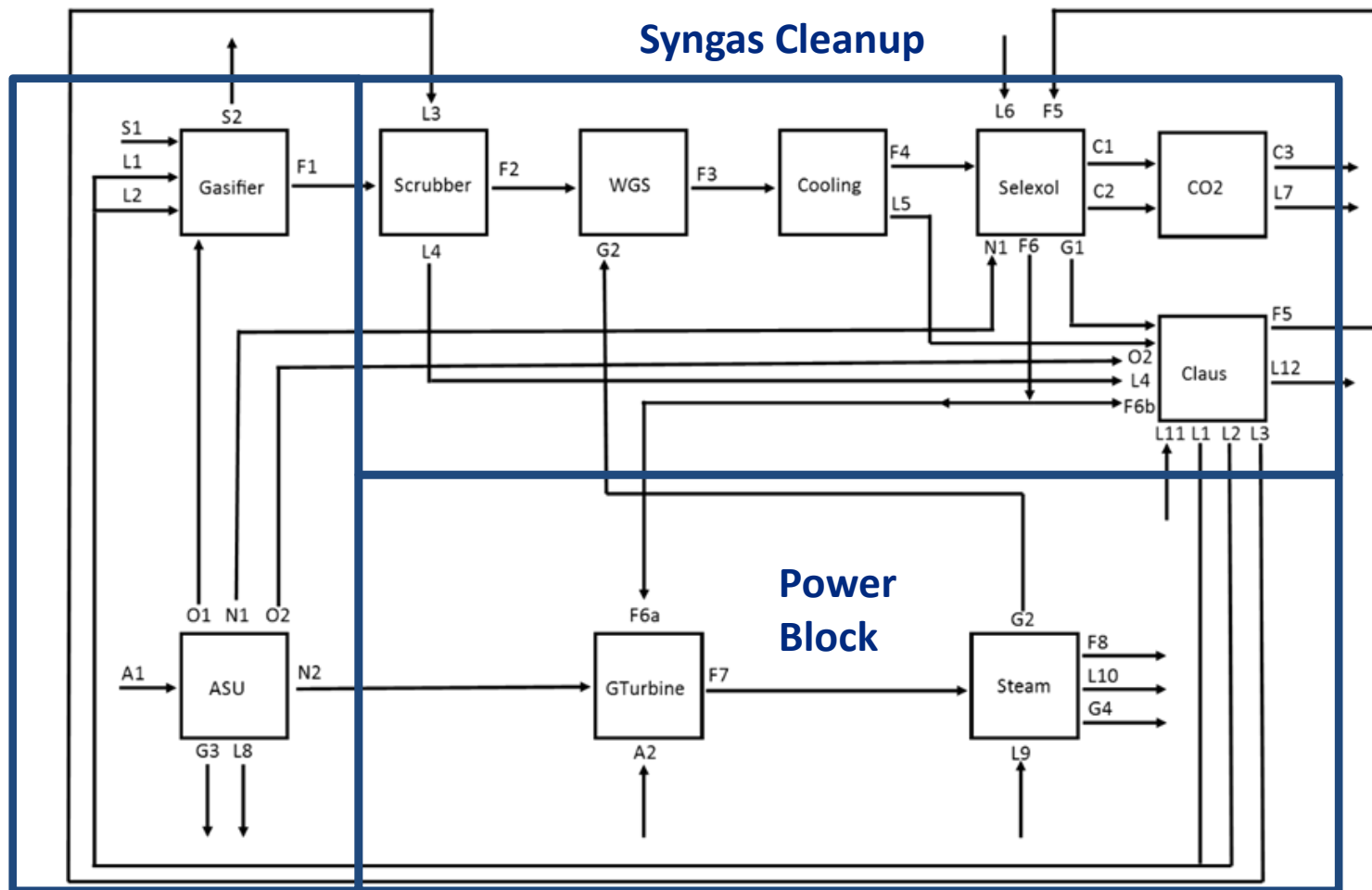
Exergy of Heat 
$$\dot{E}_j = \dot{Q}_j \cdot \left[ 1 - \frac{T_{env}}{T_{j,o} - T_{j,i}} \ln \left( \frac{T_{j,o}}{T_{j,i}} \right) \right]$$



# Baseline Model: Revisited

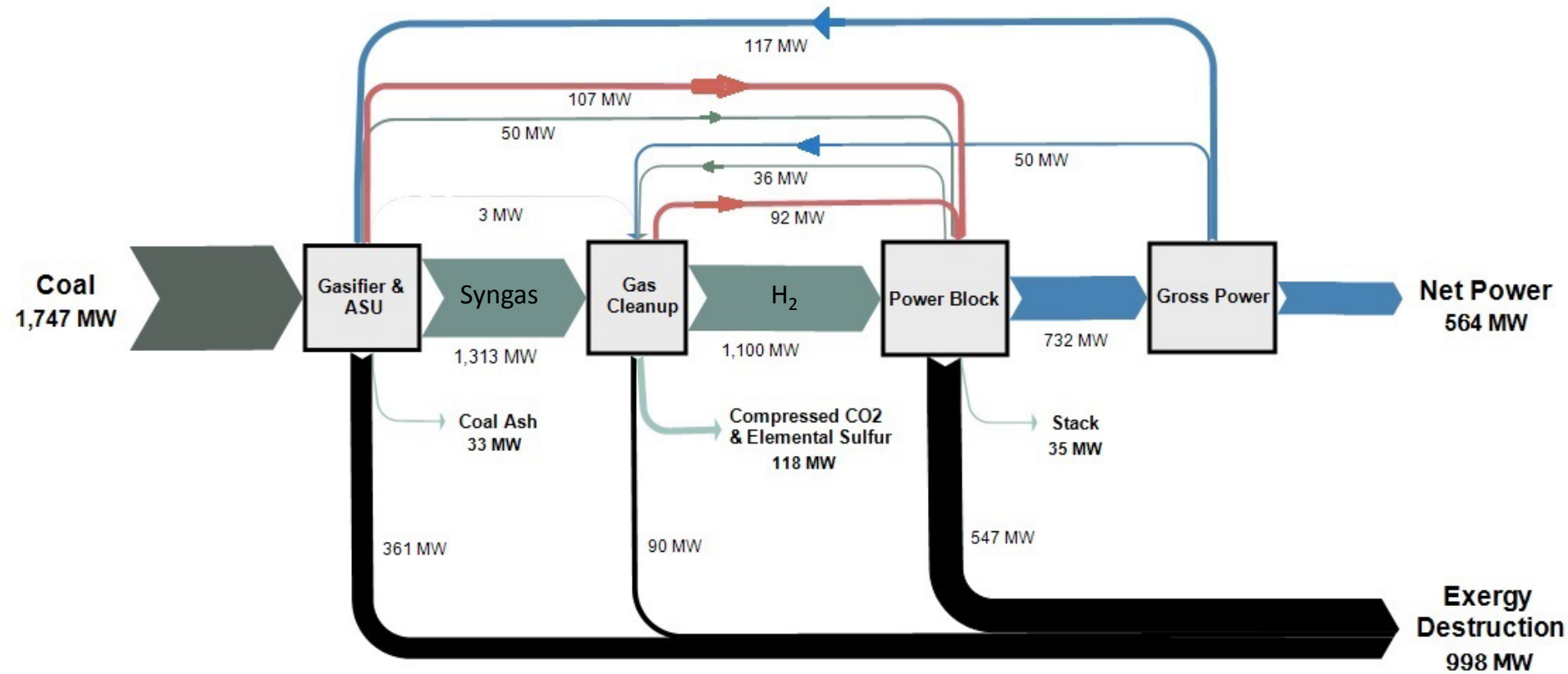


Gasifier  
+ ASU



Model #1: Baseline Model from Field and Brasington (2011)  
Based off of NETL's Bituminous Baseline Rev 2 (Nov 2010): GEE IGCC-CCS

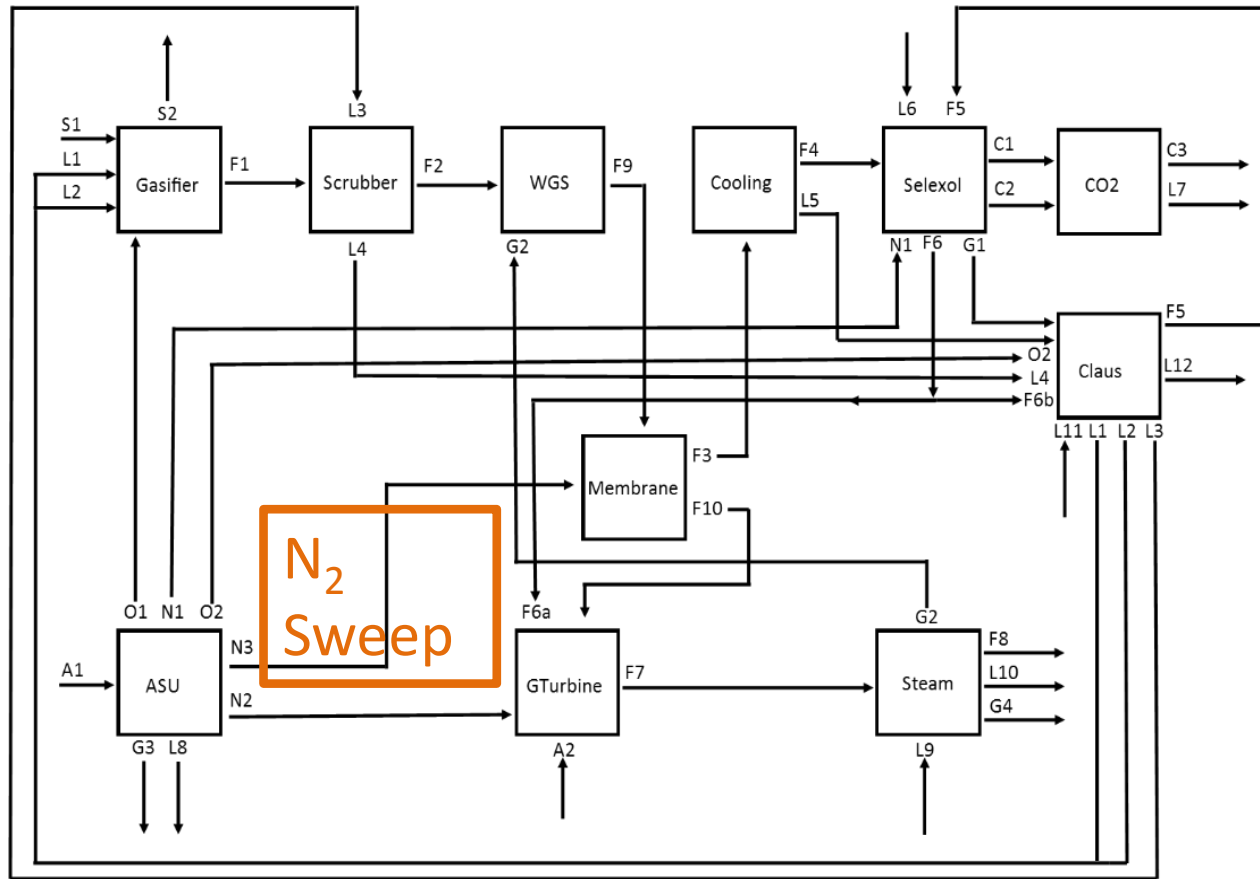
# Exergy Sankey Diagram: Baseline



- Red** = Flow of Thermal exergy between sub-systems
- Blue** = Flow of Electricity
- Teal** = Flow of Materials streams with exergy
- Black** = Exergy Destruction



# H<sub>2</sub>-Selective Membrane Model



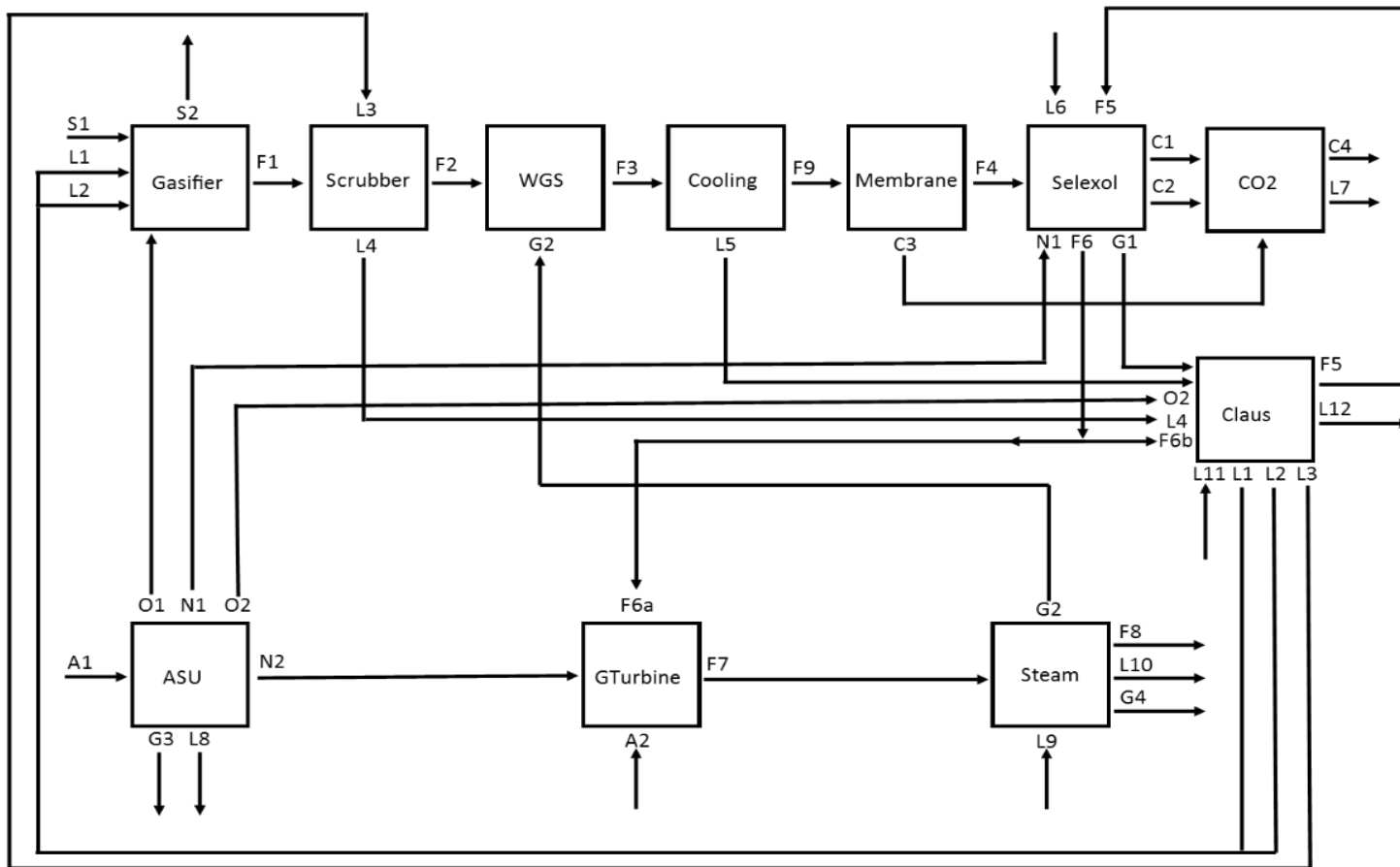
## Model #2: Hydrogen Membrane Model process flow diagram

Aspen Custom Modeler (ACM) used to model the H<sub>2</sub>-Selective Membrane

Membrane operates at 250°C. Modeled after the PBI membrane process developed by Berchtold *et. al* at LANL

H<sub>2</sub>/CO<sub>2</sub> = 48, H<sub>2</sub>/CO = 100, H<sub>2</sub>/CH<sub>4</sub> = 234, H<sub>2</sub>/H<sub>2</sub>S = 1289, H<sub>2</sub>/N<sub>2</sub> = 233, H<sub>2</sub>/H<sub>2</sub>O = 0.33

# CO<sub>2</sub>-Selective Membrane Model



## Model #3: Carbon Dioxide Membrane Model process flow diagram

Aspen Custom Modeler (ACM) used to model the CO<sub>2</sub>-Selective Membrane

Membrane operates at 40°C. Optimistic values of CO<sub>2</sub>/H<sub>2</sub> and CO<sub>2</sub>/other gases were assumed because, even at optimistic values, the process could not compete against the baseline model. CO<sub>2</sub> Selectivity was assumed to be 50 for all gases, except H<sub>2</sub>O.

# Comparison Between Cases



Subsystem or <i>Exiting Stream</i>	Baseline Model			Hydrogen Membrane Model			CO <sub>2</sub> Membrane Model		
	Norm. Power [%]	Norm. Exergy Destruction [%]	Norm. Exergy Remaining [%]	Norm. Power [%]	Norm. Exergy Destruction [%]	Norm. Exergy Remaining [%]	Norm. Power [%]	Norm. Exergy Destruction [%]	Norm. Exergy Remaining [%]
<b>Gasifier</b>	0.00	17.4	-	0.0	17.4	-	0.0	17.4	-
<b>Scrub</b>	0.00	0.2	-	0.0	0.2	-	0.0	0.2	-
<b>WGS</b>	0.00	1.3	-	0.0	1.3	-	0.0	0.2	-
<b>Mem</b>	-	-	-	0.0	0.7	-	0.0	0.2	-
<b>Cool</b>	0.00	0.0	-	0.0	0.0	-	0.0	1.1	-
<b>Selexol</b>	-1.0	2.1	-	-0.8	1.5	-	-0.4	1.0	-
<b>CO<sub>2</sub></b>	-1.6	0.4	-	-1.1	0.3	-	-1.5	0.5	-
<b>ASU</b>	-6.7	3.2	-	-5.8	3.4	-	-6.2	2.7	-
<b>GT</b>	27.0	22.6	-	26.9	21.8	-	25.2	21.5	-
<b>Steam</b>	14.8	8.8	-	14.4	8.0	-	14.7	9.3	-
<b>Claus</b>	-0.3	1.1	-	-0.2	0.8	-	-0.3	1.2	-
<i>Slag</i>		-	1.9	-	-	1.9	-	-	1.9
<i>CO<sub>2</sub> Prod</i>		-	5.0	-	-	4.9	-	-	7.8
<i>S-out</i>		-	1.7	-	-	1.6	-	-	1.6
<i>Stack Gas</i>		-	2.0	-	-	2.3	-	-	1.8
<i>Knock Out</i>		-	0.04	-	-	0.2	-	-	0.2
<b>Total</b>	<b>32.3</b>	<b>57.1</b>	<b>10.6</b>	<b>33.4</b>	<b>55.4</b>	<b>11.2</b>	<b>31.5</b>	<b>55.1</b>	<b>13.4</b>

# Summary of Results



	Baseline Model	H <sub>2</sub> -Selective Membrane Model	CO <sub>2</sub> -Selective Membrane Model
Work Produced [MW]	732.1	721.5	697.3
Work Consumed [MW]	167.8	137.2	147.4
Net Work [MW]	564.3	584.3	549.9
Total Heat Transferred to the Environment [MW <sub>th</sub> ]	799.3	686.3	759.4
CO <sub>2</sub> Captured / (CO <sub>2</sub> Capture + CO <sub>2</sub> Emitted) [%]	90.0	90.0	90.0
Hydrogen Recovered [%]	99.86	99.94	95.5
Total CO <sub>2</sub> Captured [kg/s]	128	128	128
Normalized CO <sub>2</sub> emissions [kg/MWh]	90.7	87.6	93.1

- H<sub>2</sub> membrane case increased the net efficiency compared with the baseline, whereas the CO<sub>2</sub> membrane case decreased the net efficiency
- In all cases, there was large exergy destruction in the entrained flow, quenched gasifier
  - 17.4% exergy destruction in gasifier
  - 2.4% exergy destruction in heat transfer to Rankine cycle
  - 1.9% exergy remaining in the carbon-rich slag
- From an exergy point of view, there is major room for improvement in both the gasifier and GTurbine subsystems
- Future Work: Techno-economic analyses of these 3 cases, along with a few other cases, is currently in preparation

Chen, Y., Fisher, J.C. II, Turner, M. J., Woods, M., Miller, D.C.  
“Techno-economic Analysis for H<sub>2</sub>- and CO<sub>2</sub>-selective Membranes in the Integrated Gasification Combined Cycle (IGCC) Process,” in preparation.



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**Questions?**  
**Thank you for your attention.**



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# Back Up Slides



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# Definition of Exergy & Exergy Destruction

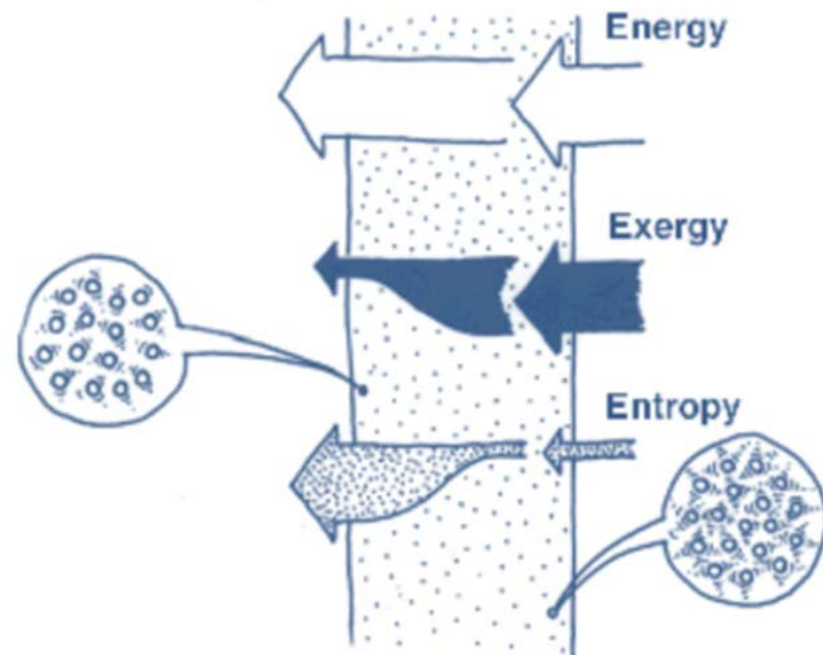


- Exergy = Maximum amount of useful work that can be obtained from a reversible process by bringing material into full mechanical, thermal, and chemical equilibrium with the environment
- Environment is usually assumed to be Earth's atmosphere at standard temperature and pressure
- Exergy cannot be negative
- Exergy can be destroyed, but not created
- All real-world processes destroy some exergy; the goal is to find the balance between low exergy destruction and low cost

$$\hat{e} = [(\hat{h} - \hat{h}_{stp}) - T_{env}(\hat{s} - \hat{s}_{stp})] + \hat{e}_{chem}$$

$$\dot{E}_j = \dot{Q}_j \cdot \left[ 1 - \frac{T_{env}}{T_{j,o} - T_{j,i}} \ln \left( \frac{T_{j,o}}{T_{j,i}} \right) \right]$$

$$\dot{\Phi}_{des} = T_{env} \cdot \dot{\sigma}_{irr}$$





# Chemical exergy of species at STP



Gas Species	Molar chemical exergy at STP [kJ/mol]	Solid Species	Molar chemical exergy at STP [kJ/mol]
N <sub>2</sub> (g)	0.69	FeO(s)	125.4
O <sub>2</sub> (g)	3.97	Fe (s)	367.6
H <sub>2</sub> O(g)	8.55	C(s)	409.8
Ar(g)	11.7	S(s) / S <sub>8</sub> (s)	75.3 / 602.7
CO <sub>2</sub> (g)	19.4	CaO/MgO	0*
H <sub>2</sub> (g)	235.2	Na <sub>2</sub> O/K <sub>2</sub> O	0*
CO(g)	274.6	Fe <sub>2</sub> O <sub>3</sub> /SiO <sub>2</sub> /Al <sub>2</sub> O <sub>3</sub>	0*
NH <sub>3</sub> (g)	336.7		
H <sub>2</sub> S(g)	804.6	<b>Liquid Species</b>	
CH <sub>4</sub> (g)	829.6	H <sub>2</sub> O(l)	0*
COS(g)	848.8	<b>* = approximation for simplicity</b>	

# Composition of reference environment at 298 K and 1 atm



Gas Species	mol%	Liquid	Activity	Solid	Activity
		H <sub>2</sub> O(l)	1	CaCO <sub>3</sub>	1
N <sub>2</sub>	75.67	NaCl(aq)	Not Appl.	CaSO <sub>4</sub> ·2H <sub>2</sub> O	1
O <sub>2</sub>	20.35			SiO <sub>2</sub>	1
H <sub>2</sub> O(g)	3.03			Al <sub>2</sub> O <sub>3</sub>	1
Ar	0.91			Fe <sub>2</sub> O <sub>3</sub>	1
CO <sub>2</sub>	0.04				

# Assumption in All Three Cases



Gas Turbine		Steam		Additional Information	
Turbine Inlet	1185°C	HP Inlet	12.5 MPa	$\eta_{\text{pump}}$	75.0-100%
Turbine Outlet	0.105 MPa	MP Inlet	6.00 MPa	$\eta_{\text{comp}}$	73.5-85%
Comp. Outlet	1.62 MPa	IP Inlet	2.90 MPa	EOS	PR-BM
$T_{\text{fuel}}$	180°C	NP Inlet	1.73 MPa	EOS- Selexol	PC-Saft
$P_{\text{fuel}}$	3.17 MPa	LP Inlet	0.45 MPa	Steam Table	STEAMNBS
$\eta_{\text{comp,isen}}$	86.5%	$\eta_{\text{isen}}$	87.5%	CO <sub>2</sub> pipeline pressure	15.3 MPa
$\eta_{\text{comp,mech}}$	98.5%	$\eta_{\text{mech}}$	98.3%	Gasifier	
$\eta_{\text{turb,isen}}$	89.8%	$\eta_{\text{pump}}$	82.0%	Pressure	5.6 MPa
$\eta_{\text{turb,mech}}$	98.8%	Condenser	0.007 MPa	Outlet T	1370°C

# Baseline Model: Results



Subsystem	Gasifier	Scrub	WGS	Cool	Selexol	CO <sub>2</sub>	ASU	GT	Steam	Claus	Total
Power [MW]	0.0	0.0	0.0	0.0	-16.7	-28.3	-117.4	472.6	259.5	-5.4	564.3
Thermal Energy Transferred to Env [MW <sub>th</sub> ]	16.9	0.0	0.3	7.7	51.6	51.3	140.3	15.5	454.3	61.4	799.3
Exergy Destroyed [MW]	304.6	4.1	22.2	0.7	36.3	7.5	56.2	394.2	153.2	19.5	998.5
Exergy in Heat To/From Steam Subsystem [MW]	122.2	0.0	80.4	14.1	-7.1	0.0	-15.4	-8.1	-190.3	4.3	0.0
Normalized Power [%]	0.0	0.0	0.0	0.0	-1.0	-1.6	-6.7	27.0	14.8	-0.3	32.3
Normalized Exergy Destruction [%]	17.4	0.2	1.3	0.04	2.1	0.4	3.2	22.5	8.8	1.1	57.1
<i>Outlet Stream</i>	<i>Slag</i>	–	–	–	–	<i>CO<sub>2</sub> Prod</i>	<i>Knock Out</i>	–	<i>Stack Gas</i>	<i>S-out</i>	
Exergy Remaining [MW]	33.0					87.4	0.7		34.2	30.2	185.6
Normalized Exergy Remaining [%]	1.9					5.0	0.0		2.0	1.7	10.6
<b>Total</b>											<b>100.0</b>

# H<sub>2</sub>-Selective Membrane: Results



Subsystem	Gasifier	Scrub	WGS	Mem	Cool	Selexol	CO <sub>2</sub>	ASU	GT	Steam	Claus	Total
Power [MW]	0.0	0.0	0.0	0.0	0.0	-13.2	-19.5	-101.5	470.1	251.4	-3.0	584.3
Thermal Energy Transferred to Env [MW <sub>th</sub> ]	16.9	0.0	0.0	0.0	5.6	38.4	41.9	127.7	15.6	405.9	34.3	686.3
Exergy Destroyed [MW]	304.6	4.1	22.8	12.4	0.8	26.2	5.3	59.4	381.0	140.6	14.7	972.0
Exergy in Heat To/From Steam Subsystem [MW]	122.2	0.0	42.8	3.9	6.8	-5.5	0.0	0.0	-3.8	-160.8	5.5	0.0
Normalized Power [%]	0.0	0.0	0.0	0.0	0.0	-0.8	-1.1	-5.8	26.9	14.4	-0.2	33.4
Normalized Exergy Destruction [%]	17.4	0.2	1.3	0.7	0.0	1.5	0.3	3.4	21.8	8.0	0.8	55.6
<i>Outlet Stream</i>	<i>Slag</i>	–	–	–	–	–	<i>CO<sub>2</sub> Prod</i>	<i>Knock Out</i>	–	<i>Stack Gas</i>	<i>S-out</i>	
Exergy Remaining [MW]	33.0						86.3	3.6		40.5	28.5	192.0
Normalized Exergy Remaining [%]	1.9						4.9	0.2		2.3	1.6	11.0
<b>Total</b>												<b>100.0</b>

# H<sub>2</sub>-Selective Membrane: Results



Subsystem	Gasifier	Scrub	WGS	Mem	Cool	Selexol	CO <sub>2</sub>	ASU	GT	Steam	Claus	Total
Power [MW]	0.0	0.0	0.0	0.0	0.0	-7.4	-26.7	-107.7	440.9	256.4	-5.7	549.9
Thermal Energy Transferred to Env [MW <sub>th</sub> ]	16.9	0.0	0.0	0.0	7.6	28.3	39.3	99.7	15.2	490.8	61.6	759.4
Exergy Destroyed [MW]	304.6	4.1	4.2	3.9	18.6	17.3	8.3	47.0	375.9	162.4	20.7	967.2
Exergy in Heat To/From Steam Subst. [MW]	122.2	0.0	80.4	0.0	14.1	-4.2	0.0	-3.3	-7.5	-205.5	3.9	0.0
Normalized Power [%]	0.0	0.0	0.0	0.0	0.0	-0.4	-1.5	-6.2	25.2	14.7	-0.3	31.5
Normalized Exergy Destruct. [%]	17.4	0.2	0.2	0.2	1.1	1.0	0.5	2.7	21.5	9.3	1.2	55.2
<i>Outlet Stream</i>	<i>Slag</i>	–	–	–	–	–	<i>CO<sub>2</sub> Prod</i>	<i>Knock Out</i>	–	<i>Stack Gas</i>	<i>S-out</i>	
Exergy Remaining [MW]	33.0						136.0	2.9		31.3	28.1	231.3
Normalized Exergy Remaining [%]	1.9						7.8	0.2		1.8	1.6	13.3
<b>Total</b>												<b>100.0</b>