Mathematical Models of Thermal Energy Storage (TES) for use with Coal FIRST Power Plants

Phase 1 Final Review

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Anoop Mathur
Anoop.Mathur@terraforetechnologies.com
951-313-6333

Joshua Schmitt

Agenda

- ☐ Introduction – team members
- ☐ Objective and Scope for Phase 1
- ☐ Status of Proposed Work Plan
- ☐ Models Implemented in IDAES
    - ☐ Three TES Technologies
    - ☐ Indirect sCO2 Power Cycle
- ☐ Results
- ☐ Plans for Phase 2

TEAM MEMBERS

MR. ANOOP MATHUR (PI)

DR. RICHARD EVANS

MR. JOSHUA SCHMITT

MR. BRANDON RIDENS

Objective for Phase 1

Implement the mathematical models for Thermal Energy Storage and Indirect sCO2 Power Plant Cycles on the IDAES Platform

Project Scope for Math Models on IDAES

- TES Models on IDAES
  - Replicate on IDAES platform math models for
    - Two-tank Sensible Heat storage in liquid(s)
    - Dual-Media Thermocline heat storage (solid & liquid)
    - Cascaded Phase Change Material heat storage (solid ⟺ liquid)
  - Add the properties library for typical heat transfer fluids and heat storage media
- sCO2 Power Cycle Model on IDAES
  - Replicate on IDAES platform math models for FPO and Indirect sCO2 Coal FIRST Cycles
    - Validate process models with multiple fuels
    - Establish optimum point for heat energy storage

Work Plan, Status

(Green complete, Red In Progress)

- Task 1. Develop Requirements
  - (Learn) IDAES platform requirements and specification
  - Plant designs inputs, outputs, constraints, assumptions, properties,…
  - Typical size of power plants, operating scenarios
  - Dynamic requirements for ancillary services
- Task 2 Replicate / Enhance Models
  - Enhance / Transfer the existing mathematical models of TES and Advanced Fossil FIRST Energy plants to IDAES Platform
  - Compare outputs from existing models of TES in Matlab and Coal FIRST in Aspen, NPSS
  - Expand the property library for heat transfer fluids and storage media, power cycle working fluids
- Task 3 Implement and test in IDAES Platform
  - Test individual models and integrate TES and power plant model
  - Run an example case with a TES and a Coal FIRST s-CO2 cycle

TES Models & Properties of HTF/ Storage Media

Thermal Energy Storage Models in Python (IDAES)	Stored Heat	HTF / Media Properties*	Ready to use for Temperature Range
"Two-Tank" Sensible Heat Storage (Current)	Sensible Heat	Various Liquids	200C to 700C
Dual-Media Thermocline Storage	Sensible Heat	Various solids and Liquids	200C to 700C
Dual Media Thermocline (actively Managed)	Sensible Heat	Various solids and Liquids	200C to 700C
Cascaded Packed Bed Phase Change Storage	Phase Change	Three PCMs salts *	280C to 550C

***Property Packages to be Included**

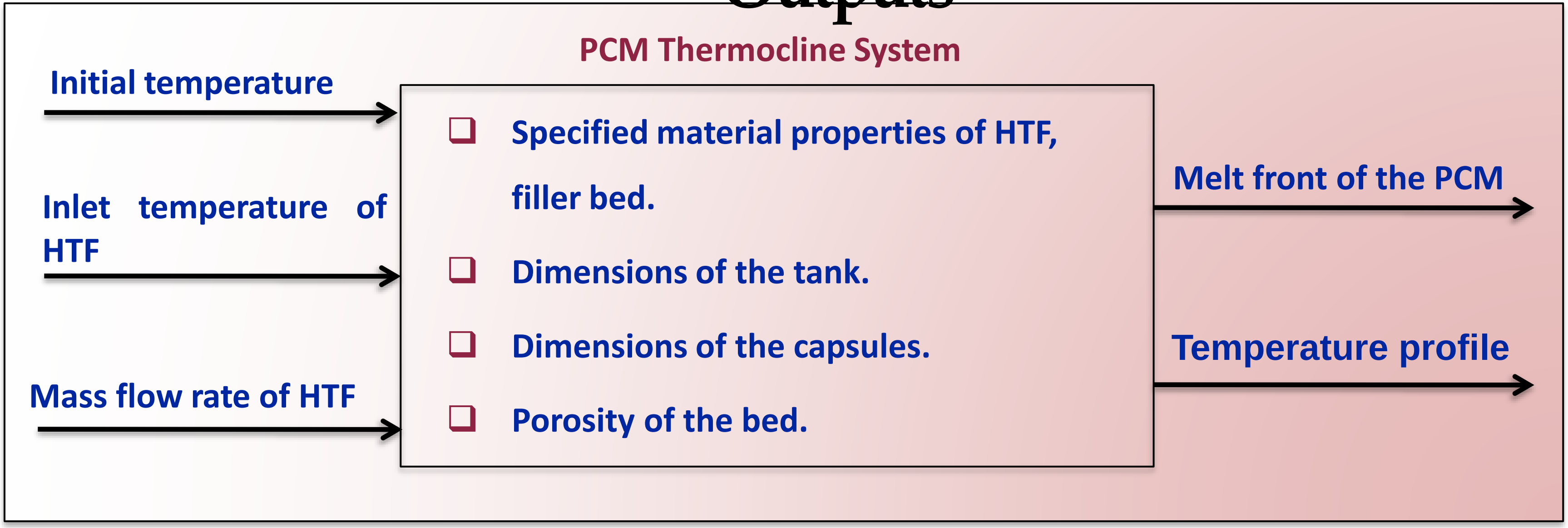
Liquids : Dowtherm, Therminol, Molten Salts (Chloride salts, Nitrate Salts)

Solids: Granite, Quartzite, 2 other solids

Three PCMs: Melting points 310 C, ~450C, 510C

Example of TES Modeling

Packed Bed Phase Change Model Inputs and Outputs



PCM Thermocline System

Initial temperature

Inlet temperature of HTF

Mass flow rate of HTF

- ☐ **Specified material properties of HTF, filler bed.**
- ☐ **Dimensions of the tank.**
- ☐ **Dimensions of the capsules.**
- ☐ **Porosity of the bed.**

Melt front of the PCM

Temperature profile

- ☐ **Identification of performance metrics**

Utilization

$$U = \frac{Q_{Discharged}}{Q_{Stored}}$$

Charging Efficiency

$$\eta = \frac{Q_{Stored}}{Q_{Input} + Q_{Pump}}$$

Discharging Efficiency

$$\eta = \frac{Q_{Output}}{Q_{Stored} + Q_{Pump}}$$

$$Q_{Output} = \int_{t_1}^{t_2} \dot{m} C_f \left(T_{f,out} - T_l\right).dt \qquad Q_{Pump} = \int_{t_1}^{t_2} \frac{\dot{m}\,\Delta p}{\rho_f}.dt$$

$$Q_{Input} = \int_{0}^{t} \dot{m} C_f \left(T_h - T_l\right).dt$$

❖ Wu et al., K.G.T., 1998, *J. Heat Transfer*

$$\Delta p = \frac{\rho_f f_s V^2 H}{\rho_{char}}; 1 \le Re \le 10^4$$

Example Equations
TES Dynamics for Packed Bed of PCM Capsules

$$\frac{\partial \phi}{\partial \tau} = -(\frac{1}{\lambda})\frac{\partial \phi}{\partial x} + (\frac{1}{Pe_{sx}})\frac{\partial^2 \phi}{\partial x^2} - (\frac{NTU}{\lambda})(\theta - \varphi)$$

$$\frac{\partial \mathrm{H}}{\partial \tau} = (\frac{NTU}{\lambda})(\theta - \varphi) + (\frac{k_{sx}/k_{fx}}{Pe_{sx}})\frac{\partial^2 \theta}{\partial x^2}$$

When,

$\mathrm{H} \geq (1 + St), \phi = (\mathrm{H} - St), \varsigma = 1(Liquid)$

$\mathrm{H} \leq (1 + St), \phi = \Phi_f, 0 \leq \zeta \leq 1$

$\mathrm{H} \leq \Phi_f, \phi = \mathrm{H}, \zeta = 0(solid)$

$$\Phi_f = \frac{T_{MPt} - T_C}{T_H - T_C}, St = \frac{H_{fusion}}{C_s(T_H - T_C)}$$

For Cascaded PCM

$$x \leq \frac{L_1}{L}, then, H_{fusion} = H_{salt1}, T_{MPt} = T_{salt1}$$

$$\frac{L_1}{L} < x \leq \frac{L_2}{L}, then, H_{fusion} = H_{salt2}, T_{MPt} = T_{salt2}$$

$$\frac{L_2}{L} < x \leq 1, then, H_{fusion} = H_{salt3}, T_{MPt} = T_{salt3}$$

Boundary Conditions for Charging and Discharging

$x = 0, \theta = 0$	$x = 1, \theta = 1$
$x = 1, \frac{\partial \theta}{\partial x} = 0, \frac{\partial \phi}{\partial x} = 0$	$x = 0, \frac{\partial \theta}{\partial x} = 0, \frac{\partial \phi}{\partial x} = 0$
$\tau \leq 0, 0 \leq x \leq 1, \mathrm{H}\ \&\ \theta, \zeta, specifiedprofile$	$\tau \leq 0, 0 \leq x \leq 1, \phi\ \&\ \theta specifiedprofile$

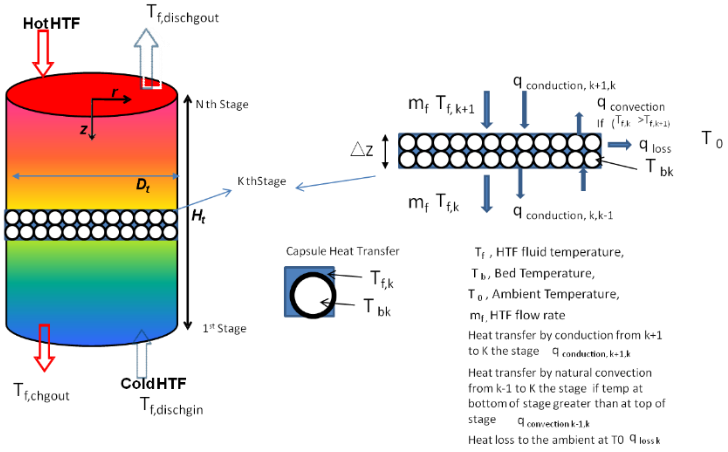
Dimensionless Variables

$$\theta = \frac{(T_f - T_C)}{(T_H - T_C)}, \phi = \frac{(T_s - T_C)}{(T_H - T_C)}, H = \frac{\left[C_s(T_s - T_C) + \zeta H_{fusion}\right]}{C_s(T_H - T_C)}$$

$$x = \frac{z}{L}, Pe_x = \frac{GC_f L}{k_{fx}}, NTU = \frac{h_v L}{GC_f},$$

$$\lambda = \frac{\varepsilon \rho_f C_f}{(1-\varepsilon)\rho_s C_s + \varepsilon \rho_f C_f}$$

$$\tau = \frac{GC_f t}{\left[(1-\varepsilon)\rho_s C_s + \varepsilon \rho_f C_f\right]}\left[\frac{1}{L}\right]$$



T_f, HTF fluid temperature,

T_b, Bed Temperature,

T_0, Ambient Temperature,

m_f, HTF flow rate

Heat transfer by conduction from k+1 to K the stage $q_{conduction, k+1,k}$

Heat transfer by natural convection from k-1 to K the stage if temp at bottom of stage greater than at top of stage $q_{convection\ k-1,k}$

Heat loss to the ambient at T0 $q_{loss\ k}$

Level of Sophistication Models

- Level of sophistication models designed to capture key attributes of TES* to efficiently run power plant model for
  - Optimization of TES size, Diurnal Simulation
- Dynamic model of HX is adequate to evaluate TES* systems for
  - Dispatchability, Ramp-up & down
  - Power Cycle Operation (charge rate & discharge rate)

*Solid media storage such as in Concrete may require detailed models

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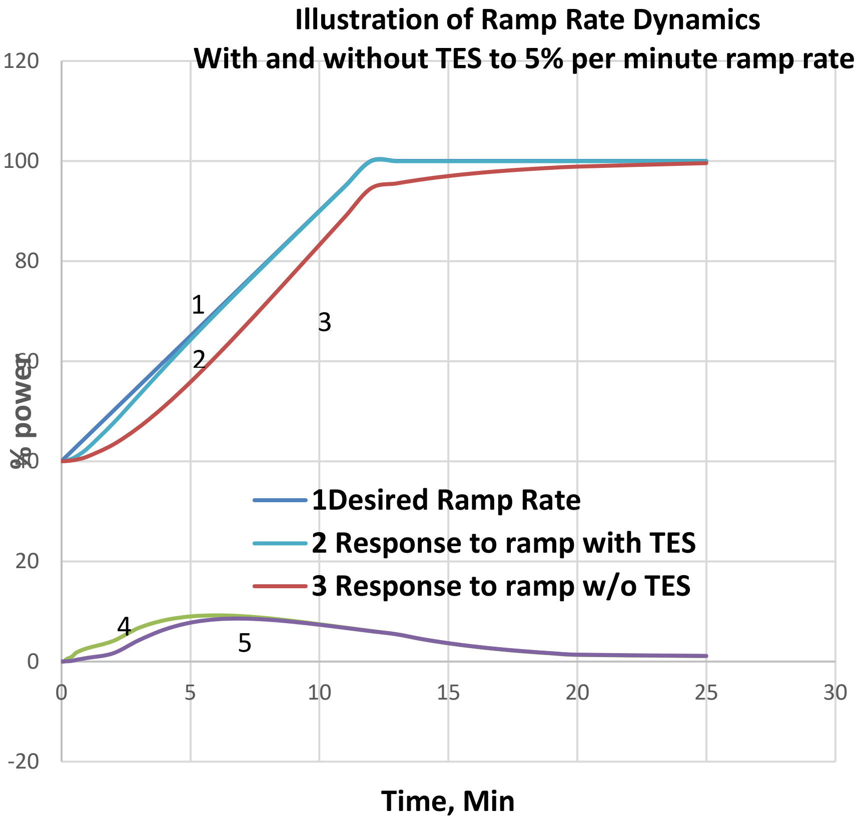
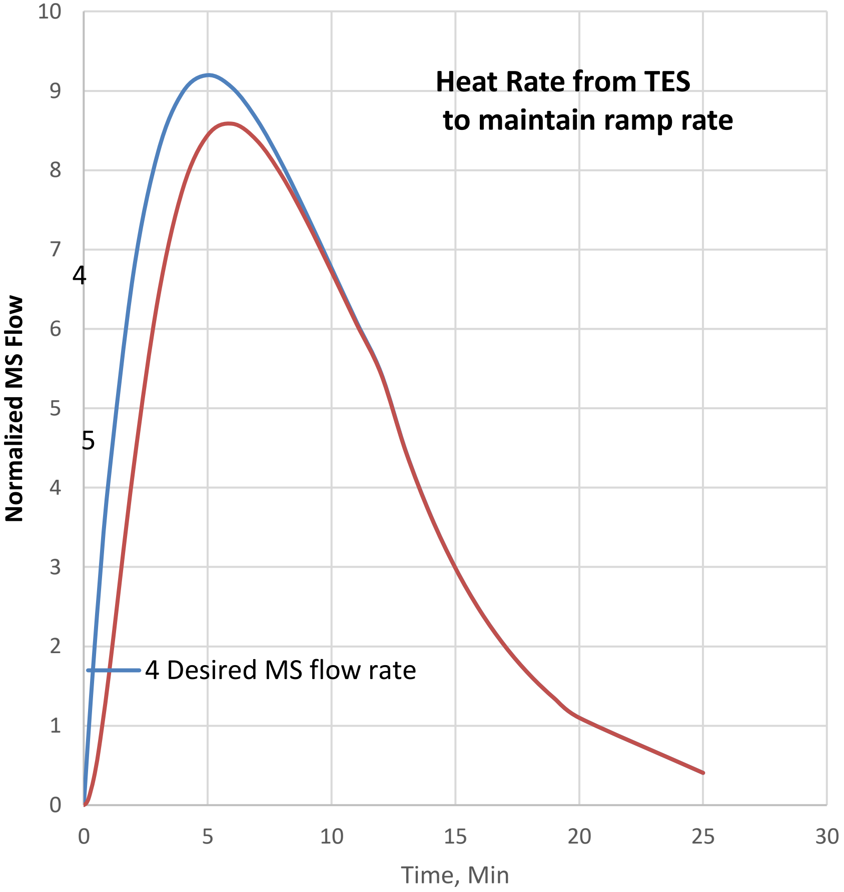
Important TES Attributes

- Discharge Temperature Profile
- Energy Density
- Rate of Change of Temperature during ramp-up and ramp-down
- Conversion efficiency, & Ramp rate
- Cost of TES & Footprint
- Metal stress and life of plant

Example Use of TES in IDAES (Using IDAES Heater Model)





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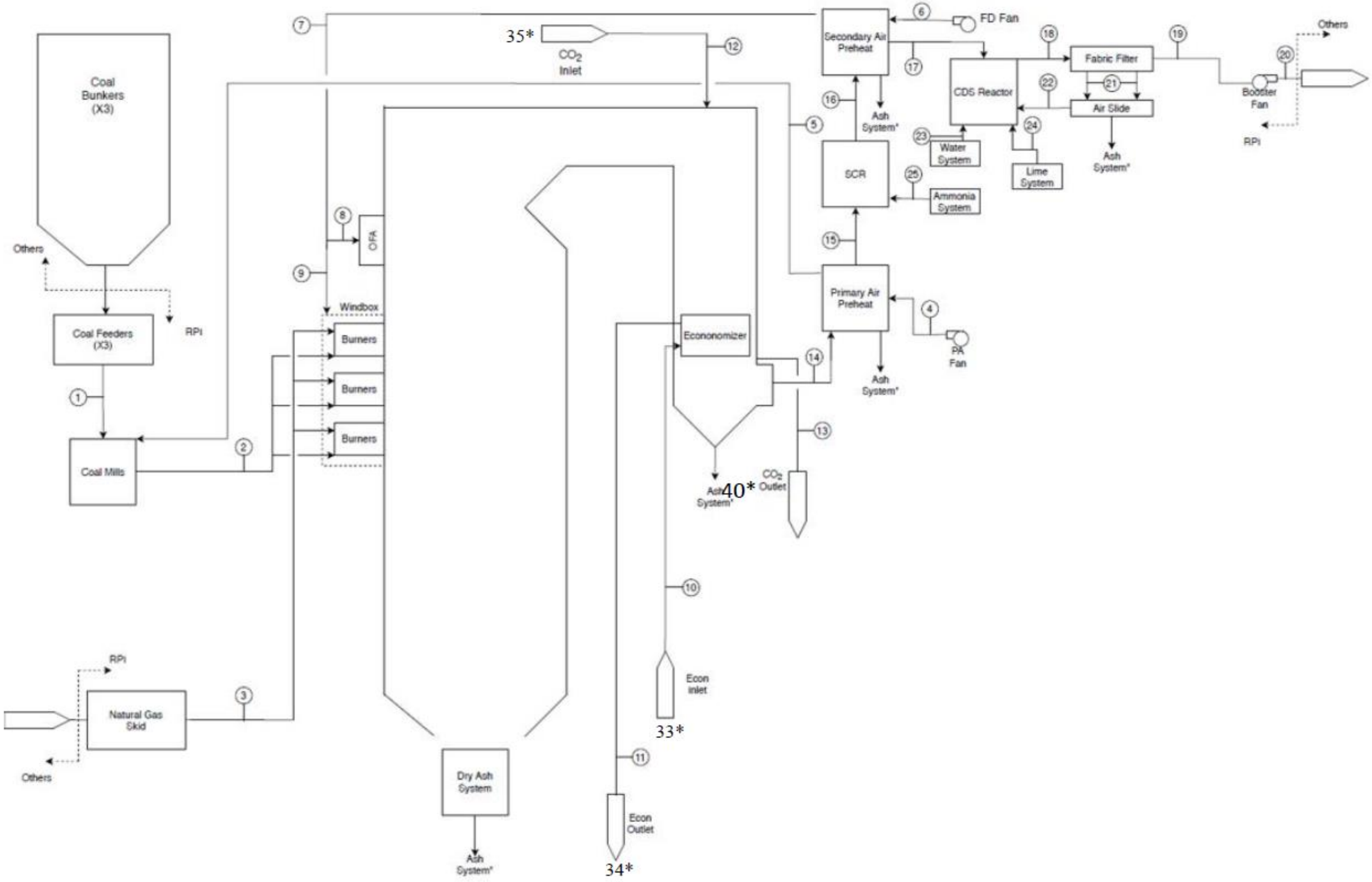
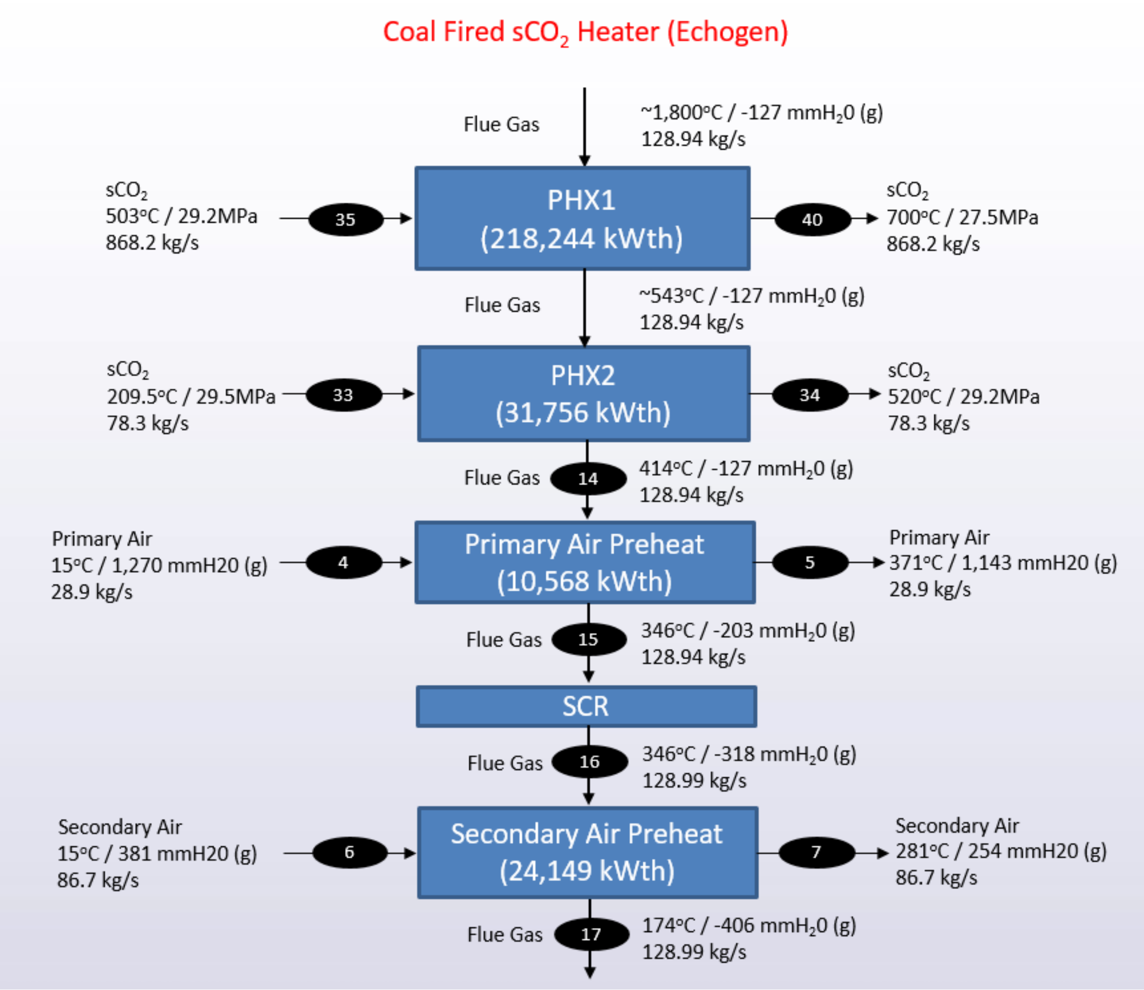
Indirect sCO2 Cycle Modeling

Block Diagram of sCO2 Fired Heater (from Echogen)



Post Combustion Flue Gas Flow Path (from Echogen)

*Echogen did not provide flue gas properties. Properties of PHX1 and PHX2 are considered approximations



Coal Fired sCO$_2$ Heater (Echogen)

Flue Gas
~1,800°C / -127 mmH$_2$0 (g)
128.94 kg/s

sCO$_2$
503°C / 29.2MPa
868.2 kg/s
35

PHX1
(218,244 kWth)

40
sCO$_2$
700°C / 27.5MPa
868.2 kg/s

Flue Gas
~543°C / -127 mmH$_2$0 (g)
128.94 kg/s

sCO$_2$
209.5°C / 29.5MPa
78.3 kg/s
33

PHX2
(31,756 kWth)

34
sCO$_2$
520°C / 29.2MPa
78.3 kg/s

Flue Gas
14
414°C / -127 mmH$_2$0 (g)
128.94 kg/s

Primary Air
15°C / 1,270 mmH20 (g)
28.9 kg/s
4

Primary Air Preheat
(10,568 kWth)

5
Primary Air
371°C / 1,143 mmH20 (g)
28.9 kg/s

Flue Gas
15
346°C / -203 mmH$_2$0 (g)
128.94 kg/s

SCR

Flue Gas
16
346°C / -318 mmH$_2$0 (g)
128.99 kg/s

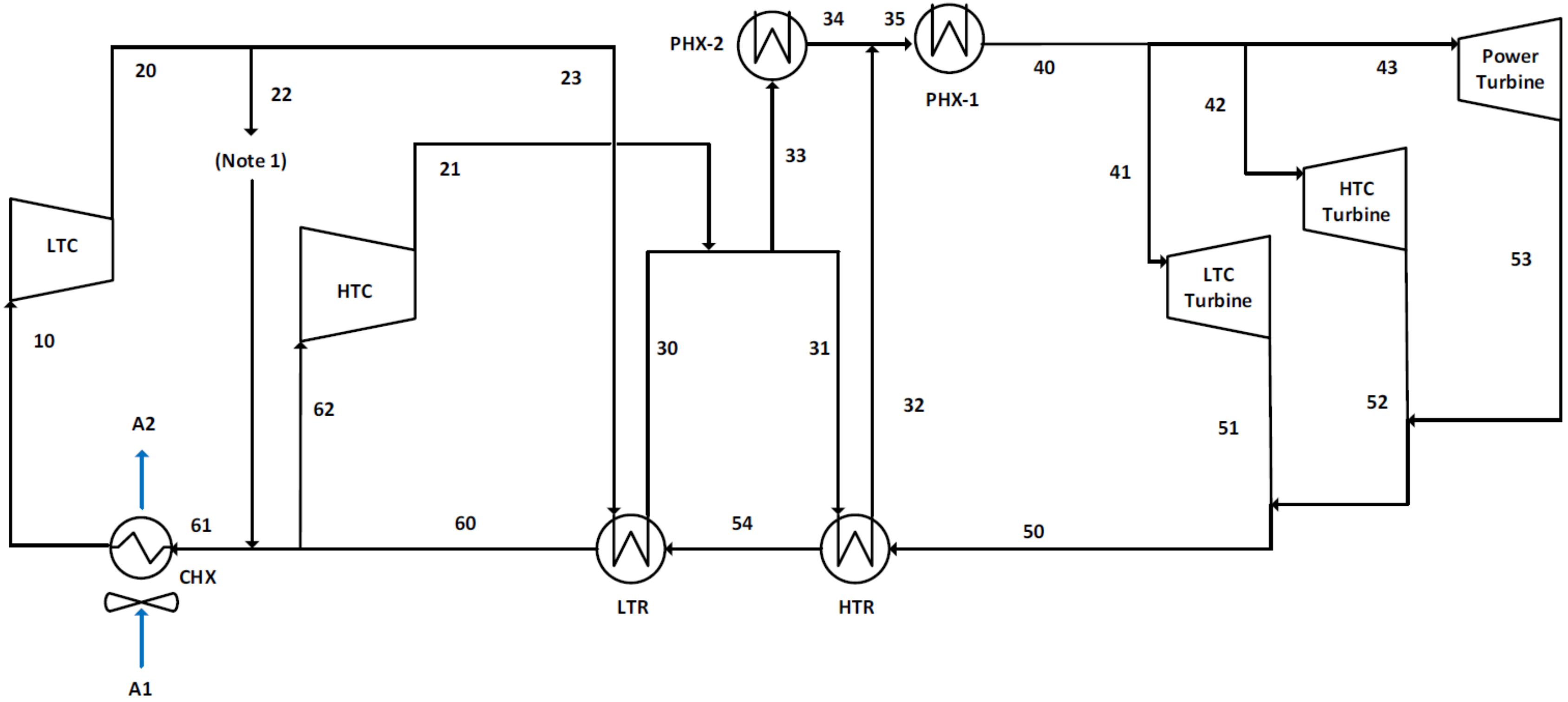
Secondary Air
15°C / 381 mmH20 (g)
86.7 kg/s
6

Secondary Air Preheat
(24,149 kWth)

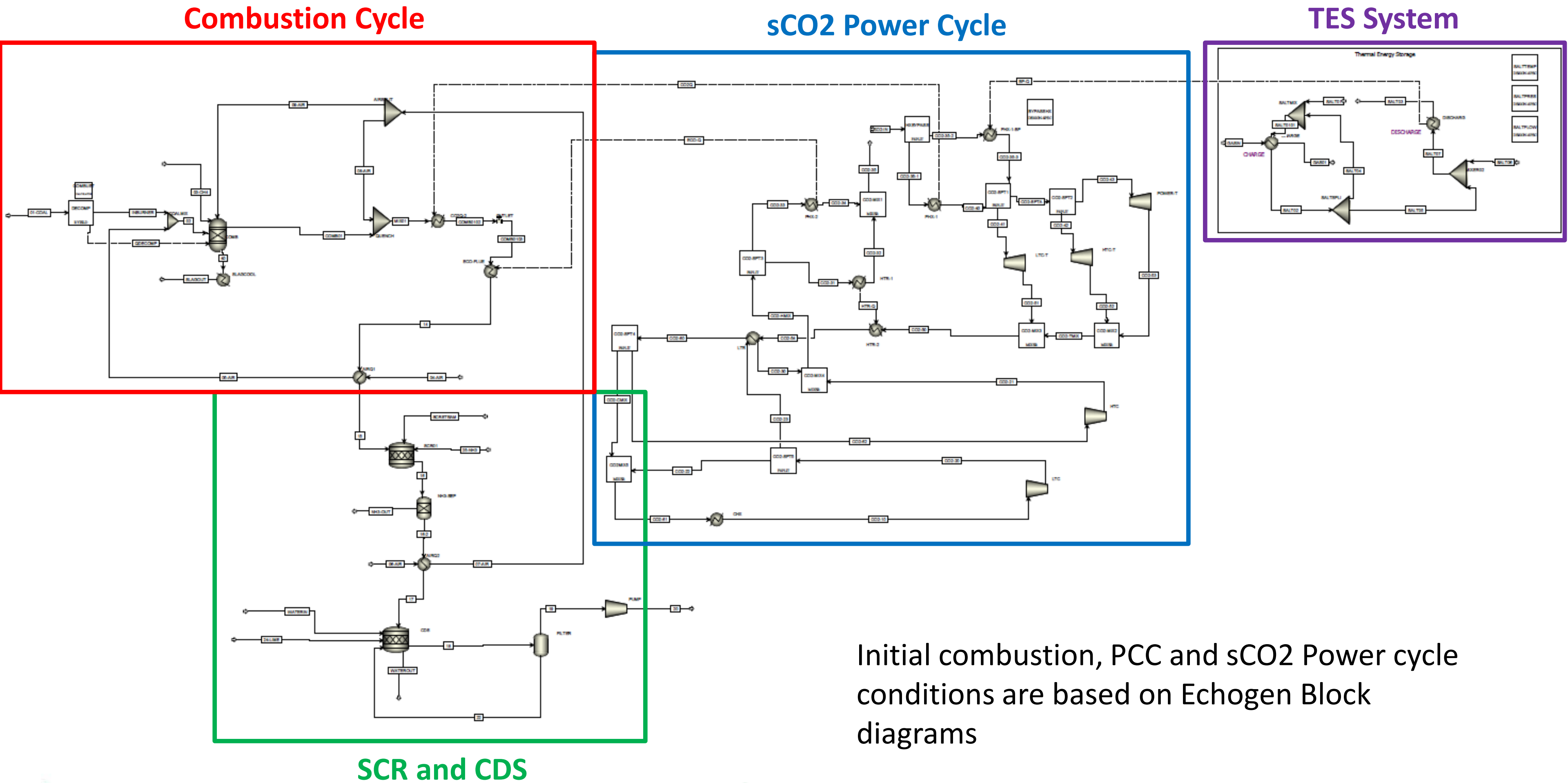
7
Secondary Air
281°C / 254 mmH20 (g)
86.7 kg/s

Flue Gas
17
174°C / -406 mmH$_2$0 (g)
128.99 kg/s

Block Diagram of sCO2 Power Cycle (from Echogen)



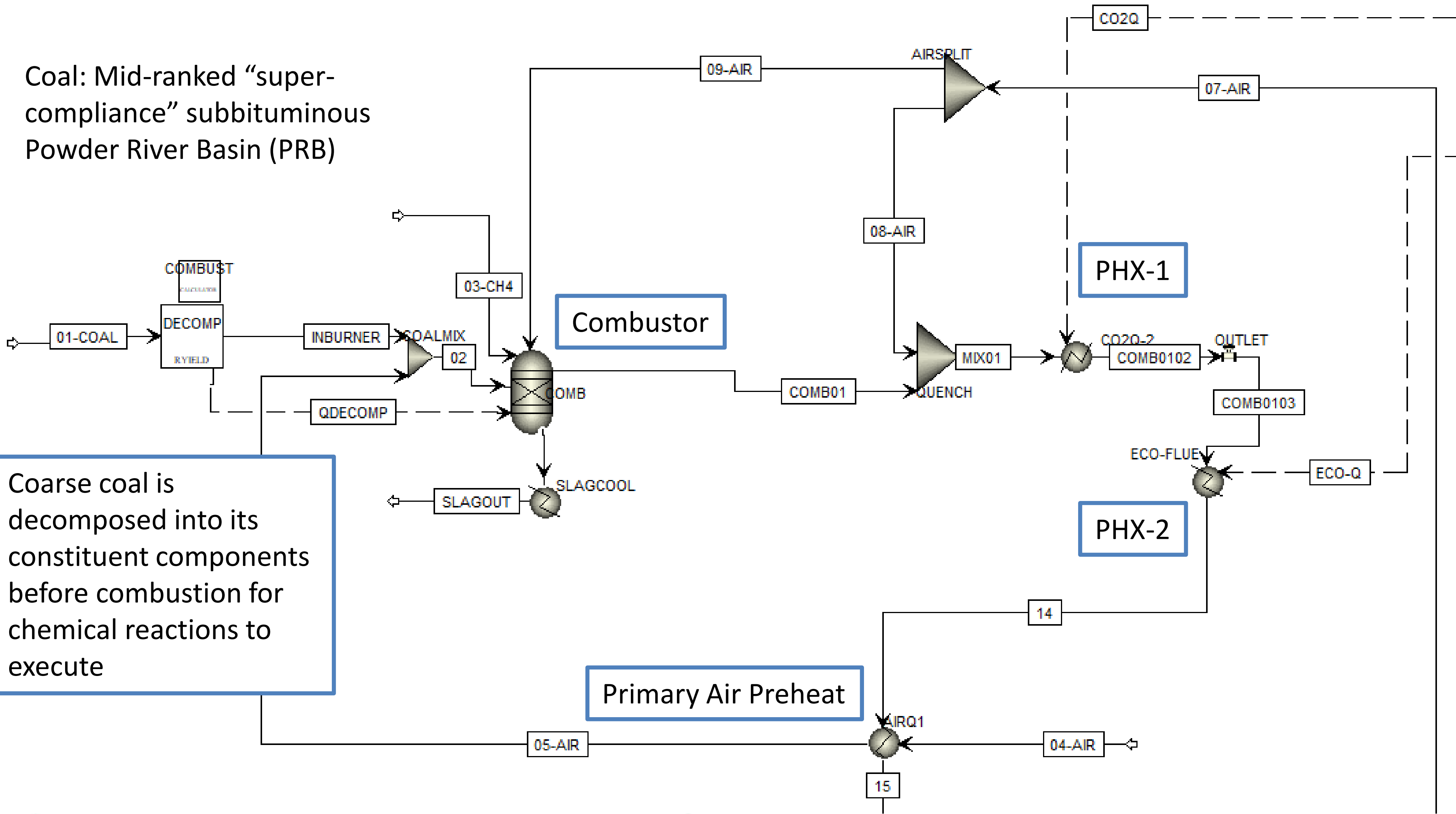
Current Aspen Plus (v10) Process Model



Initial combustion, PCC and sCO2 Power cycle conditions are based on Echogen Block diagrams

Combustion Cycle Model

Coal: Mid-ranked “super-compliance” subbituminous Powder River Basin (PRB)



Combustor

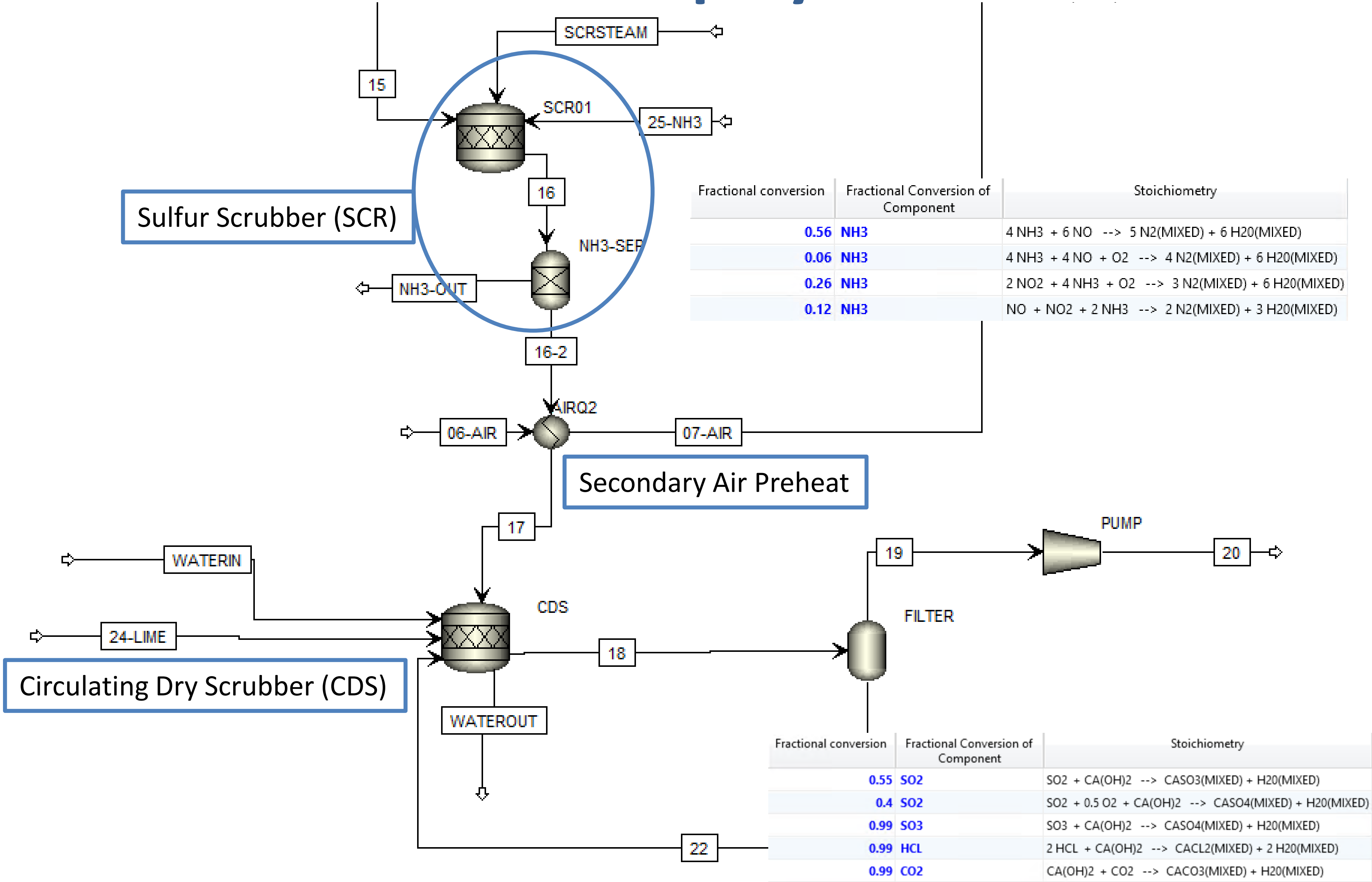
PHX-1

PHX-2

Primary Air Preheat

Coarse coal is decomposed into its constituent components before combustion for chemical reactions to execute

Flue Gas Clean Up Cycle Model



Sulfur Scrubber (SCR)

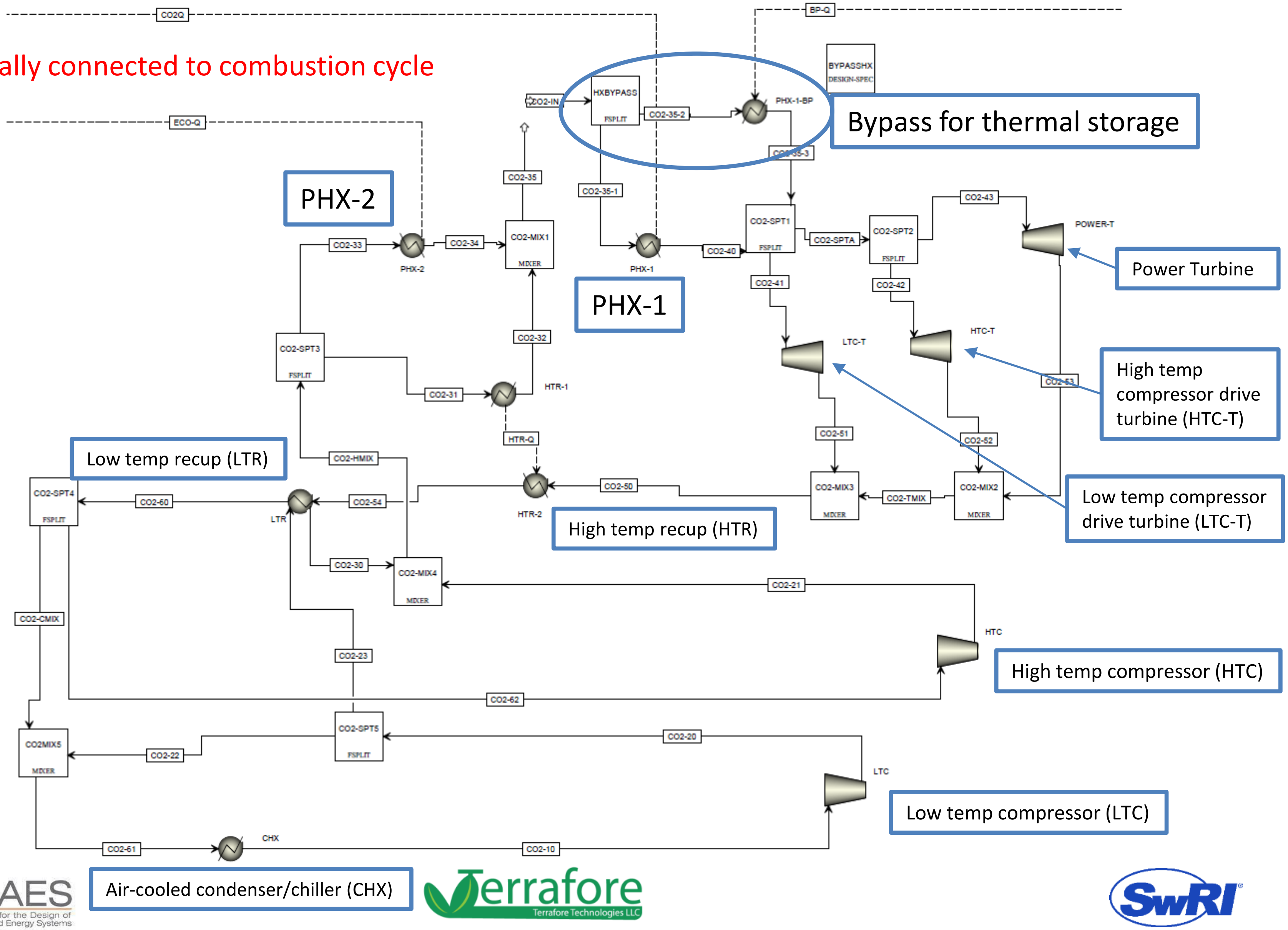
Secondary Air Preheat

Circulating Dry Scrubber (CDS)

Fractional conversion	Fractional Conversion of Component	Stoichiometry
0.56	NH3	4 NH3 + 6 NO --> 5 N2(MIXED) + 6 H20(MIXED)
0.06	NH3	4 NH3 + 4 NO + O2 --> 4 N2(MIXED) + 6 H20(MIXED)
0.26	NH3	2 NO2 + 4 NH3 + O2 --> 3 N2(MIXED) + 6 H20(MIXED)
0.12	NH3	NO + NO2 + 2 NH3 --> 2 N2(MIXED) + 3 H20(MIXED)

Fractional conversion	Fractional Conversion of Component	Stoichiometry
0.55	SO2	SO2 + CA(OH)2 --> CASO3(MIXED) + H20(MIXED)
0.4	SO2	SO2 + 0.5 O2 + CA(OH)2 --> CASO4(MIXED) + H20(MIXED)
0.99	SO3	SO3 + CA(OH)2 --> CASO4(MIXED) + H20(MIXED)
0.99	HCL	2 HCL + CA(OH)2 --> CACL2(MIXED) + 2 H20(MIXED)
0.99	CO2	CA(OH)2 + CO2 --> CACO3(MIXED) + H20(MIXED)

sCO2 Power Cycle System Model



Thermally connected to combustion cycle

Bypass for thermal storage

PHX-2

PHX-1

Power Turbine

High temp compressor drive turbine (HTC-T)

Low temp recup (LTR)

High temp recup (HTR)

Low temp compressor drive turbine (LTC-T)

High temp compressor (HTC)

Low temp compressor (LTC)

Air-cooled condenser/chiller (CHX)

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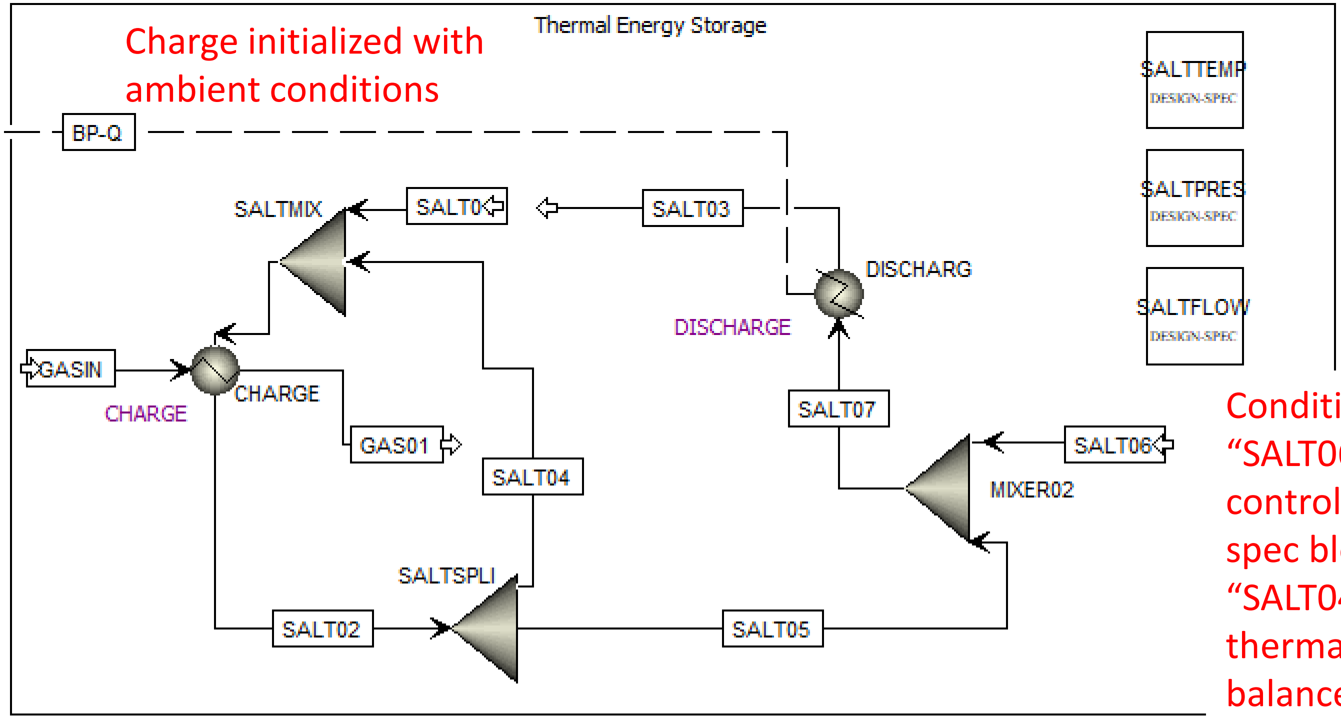
Thermal Energy Storage System (TES)

Steady state modeling with charge and discharge cycles using molten salt



Charge initialized with ambient conditions

Conditions of "SALT06" are controlled by design spec blocks to match "SALT04" to maintain thermal and mass balance

Can be tied into existing model in either charge or discharge mode

Aspen Results

Combustion and PCC Cycles

Aspen Plus Model				EPS Design Parameters			
Name	Temperature	Pressure	Mass Flow	Name	Temperature	Pressure	Mass Flow
	K	kPa	kg/sec		K	kPa (mm H2O g)	kg/sec
01-COAL	288.15	90.00	14.15	1	288.15	N/A	14.15
2	329.38	106.31	43.05	2	339.15	(508)	43.05
03-CH4	288.15	340.00	0.29	3	288.15	340	0.29
04-AIR	288.15	113.78	28.90	4	288.15	(1270)	28.90
05-AIR	626.63	112.53	28.90	5	644.15	(1143)	28.90
06-AIR	288.15	105.06	86.75	6	288.15	(381)	86.75
07-AIR	566.43	103.82	86.75	7	561.15	(254)	86.75
08-AIR	566.43	103.82	23.13	8	561.15	(254)	23.13
09-AIR	566.43	103.82	63.62	9	561.15	(254)	63.62
14	687.17	100.08	128.93	14	687.15	(-127)	128.94
15	619.15	99.33	128.93	15	619.15	(-203)	128.94
16	619.15	98.21	129.04	16	619.15	(-318)	128.99
16-2	619.15	98.21	129.02				
17	447.15	97.34	129.02	17	447.15	(-406)	128.99
18	352.15	96.10	211.73	18	352.15	(-533)	190.69
19	352.15	93.85	135.43	19	352.15	(-762)	135.58
20	359.67	101.57	135.43	20	361.15	(25)	135.58
22	352.15	93.85	75.75	22	352.15	(-406)	54.36
24-LIME	350.00	140	0.37	24	288.15	140	0.37
25-NH3	288.15	660	0.06	25	288.15	660	0.06
40	2280.56	106.31	1.16				

sCO_2 Power Cycle

Aspen Plus Model				EPS Design Parameters			
Name	Temperature	Pressure	Mass Flow	Name	Temperature	Pressure	Mass Flow
	K	kPa	kg/sec		K	kPa (mm H2O g)	kg/sec
CO2-10	294.85	6520	557.40	10	294.85	6520	568
CO2-20	323.23	30000	557.40	20	323.35	30000	568
CO2-21	474.77	29580	318.10	21	474.85	29580	318.1
CO2-22	323.23	30000	7.40	22	323.35	30000	18
CO2-23	323.23	30000	550.00	23	323.35	29970	550
CO2-30	488.40	29580	550.00	30	487.35	29580	550
CO2-31	483.36	29580	789.80	31	482.65	29500	789.9
CO2-32	774.05	29290	789.80	32	774.05	29290	789.9
CO2-33	483.36	29580	78.30	33	482.65	29510	78.3
CO2-34	793.15	29210	78.30	34	793.15	29210	78.3
CO2-35-1	775.75	29210	766.62	35	775.75	29210	868.2
CO2-35-2	775.75	29210	101.58				
CO2-35-3	973.15	27510	101.58				
CO2-40	973.15	27510.00	766.62	40	973.15	27510	868.2
CO2-41	973.13	27410.00	91.70	41	973.15	27410	91.7
CO2-42	973.13	27410	156.80	42	973.15	27410	156.8
CO2-43	973.13	27410	619.70	43	973.15	27410	619.7
CO2-50	796.71	7020	868.20	50	796.65	7020	868.2
CO2-51	804.55	7120	91.70	51	804.45	7120	91.7
CO2-52	802.45	7120	156.80	52	802.45	7120	156.8
CO2-53	794.21	7120	619.70	53	794.15	7120	619.7
CO2-54	494.67	6920	868.20	54	493.75	6920	868.2
CO2-60	333.55	6770	868.20	60	333.55	6770	868.2
CO2-61	333.27	6690	557.40	61	329.35	6690	568
CO2-62	332.93	6690	318.10	62	332.95	6690	318.1

IDAES Flowsheet and Plant Model Development

- Use property packages from existing libraries
  - Swco2
  - Flue gas
- Use integrated unit models
  - Compressor
  - Turbine
  - Pressure Changer
  - Mixer
  - Separator
  - Heater
  - Heat Exchanger
- Run in power cycle in open loop and match inlet to outlet to ensure stability

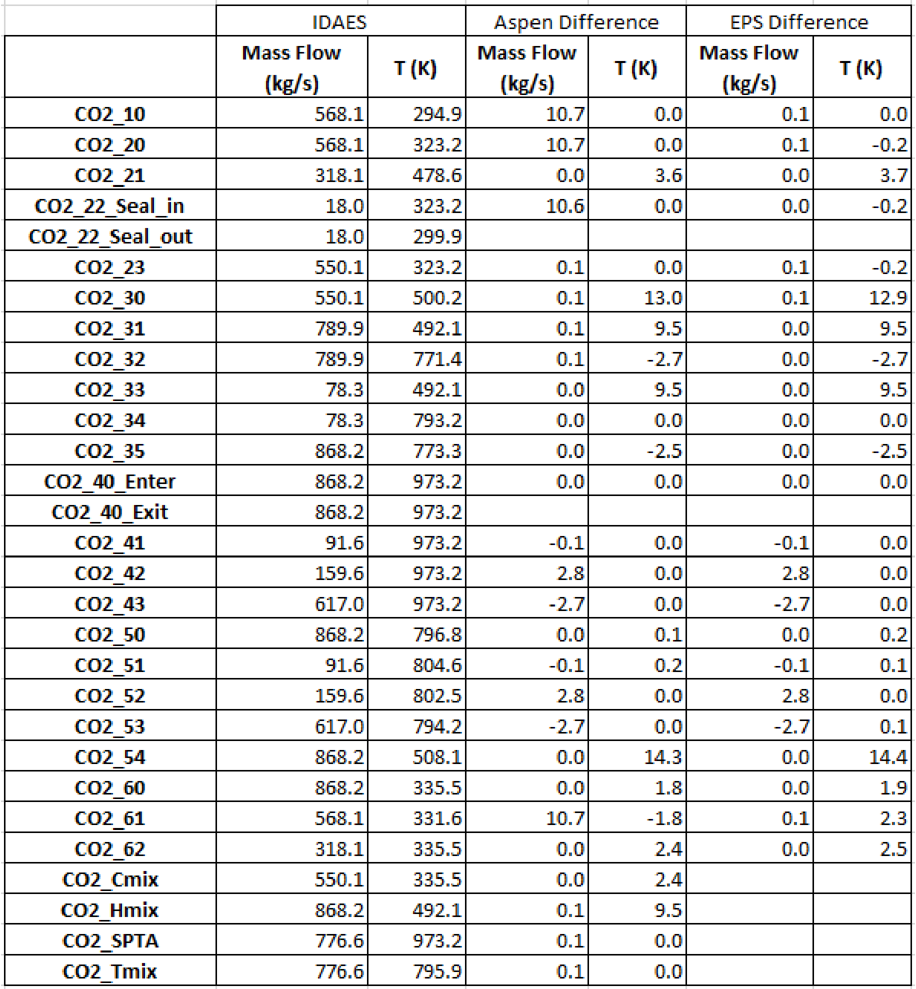
IDAES Unit Block Specified Values

Unit Model	IDAES Model Type	Fixed Property	Value
LTC	“Compressor”	Isentropic Efficiency	0.883
		Pressure Ratio	4.6012
HTC	“Compressor”	Isentropic Efficiency	0.866
		Pressure Ratio	4.4215
LTC_T	“Turbine”	Isentropic Efficiency	0.864
		Pressure Ratio	0.25976
HTC_T	“Turbine”	Isentropic Efficiency	0.875
		Pressure Ratio	0.25976
Power_T	“Turbine”	Isentropic Efficiency	0.918
		Pressure Ratio	0.25976
CHX	“Heater”	Delta Pressure	-1.7e5 Pa
PHX1	“Heater”	Delta Pressure	-1.7e6 Pa
PHX2	“Heater”	Delta Pressure	-3.0e5 Pa
HTR	“HeatExchanger”	Overall Heat Transfer Coefficient	1158.4 W/K-m^2
		Surface Area	1.2203e4 m^2
		Hot Side Delta Pressure	-1e5 Pa
		Cold Side Delta Pressure	-2.1e5 Pa
LTR	“HeatExchanger”	Overall Heat Transfer Coefficient	1855.5 W/K-m^2
		Surface Area	9596.9 m^2
		Hot Side Delta Pressure	-1.5e5 Pa
		Cold Side Delta Pressure	-3.9e5 Pa
CO2_SPT1	“Separator”	Split Fraction to CO2_41	0.1056
CO2_SPT2	“Separator”	Split Fraction to CO2_42	0.2019
CO2_SPT3	“Separator”	Split Fraction to CO2_31	0.9098
CO2_SPT4	“Separator”	Split Fraction to CO2_62	0.3664
CO2_SPT5	“Separator”	Split Fraction to CO2_23	0.9683

IDAES sCO2 Model Results

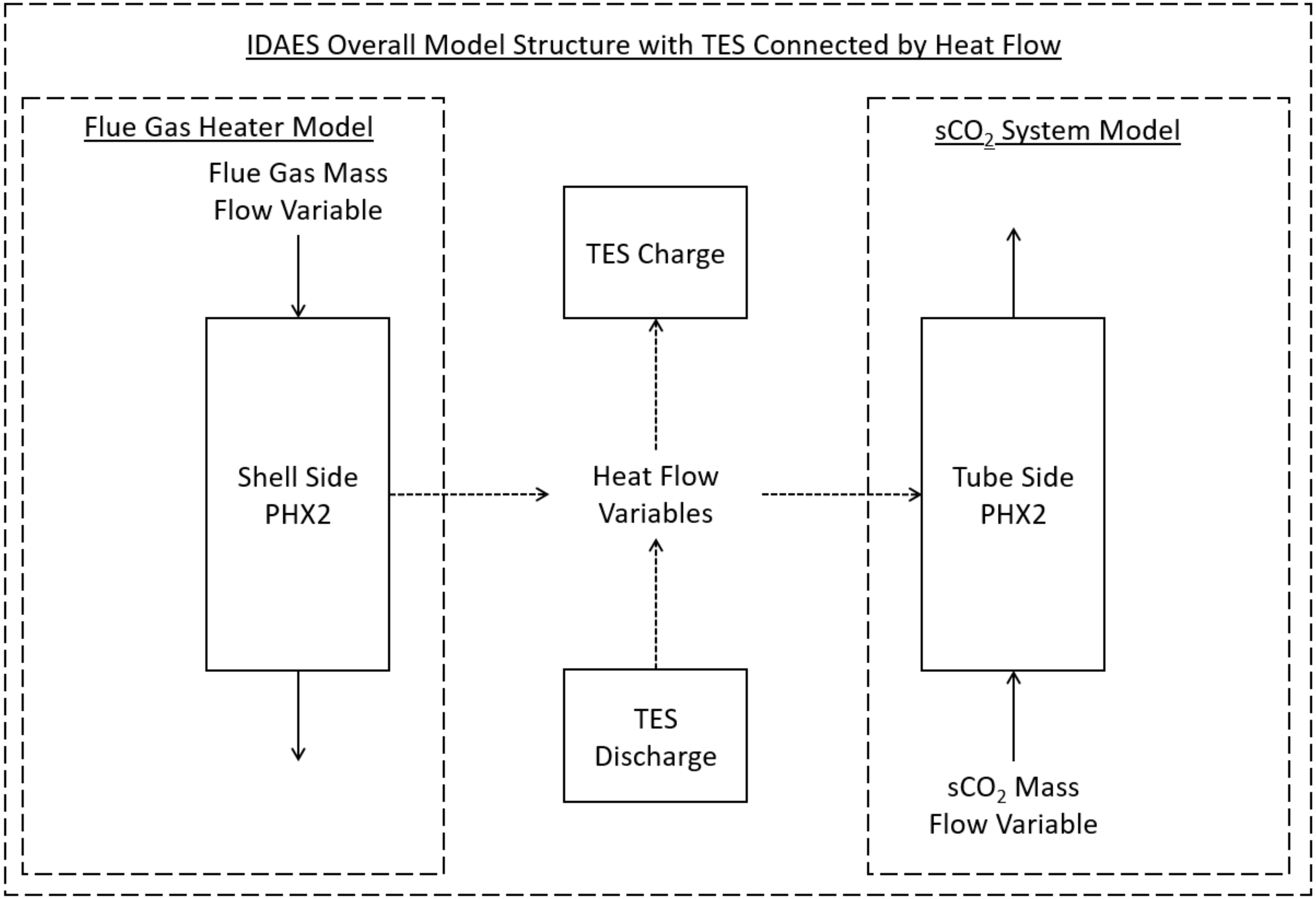
	Molar Flow (mol/s)	Mass Flow (kg/s)	T (K)	P (Pa)	Vapor Fraction	Molar Enthalpy (J/mol) Vap	Molar Enthalpy (J/mol) Liq
CO2_10	12908	568.1	294.9	6.52E+06	0	-10326.4	-10945.7
CO2_20	12908	568.1	323.2	3.00E+07	0	-9542.8	-9542.8
CO2_21	7228	318.1	478.6	2.96E+07	0	3194.0	3194.0
CO2_22_Seal_in	409	18.0	323.2	3.00E+07	0	-9542.8	-9542.8
CO2_22_Seal_out	409	18.0	299.9	6.69E+06	0.066973	-5241.1	-9851.6
CO2_23	12499	550.1	323.2	3.00E+07	0	-9542.8	-9542.8
CO2_30	12499	550.1	500.2	2.95E+07	0	4598.7	4598.7
CO2_31	17948	789.9	492.1	2.95E+07	0	4084.0	4084.0
CO2_32	17948	789.9	771.4	2.93E+07	0	20115.5	20115.5
CO2_33	1779	78.3	492.1	2.95E+07	0	4084.0	4084.0
CO2_34	1779	78.3	793.2	2.92E+07	0	21327.4	21327.4
CO2_35	19727	868.2	773.3	2.92E+07	0	20224.7	20224.7
CO2_40_Enter	19727	868.2	973.2	2.74E+07	0	31426.3	31426.3
CO2_40_Exit	19727	868.2	973.2	2.74E+07	0	31426.3	31426.3
CO2_41	2082	91.6	973.2	2.74E+07	0	31426.3	31426.3
CO2_42	3626	159.6	973.2	2.74E+07	0	31426.3	31426.3
CO2_43	14019	617.0	973.2	2.74E+07	0	31426.3	31426.3
CO2_50	19727	868.2	796.8	7.12E+06	1	22320.7	22320.7
CO2_51	2082	91.6	804.6	7.12E+06	1	22727.4	22727.4
CO2_52	3626	159.6	802.5	7.12E+06	1	22616.7	22616.7
CO2_53	14019	617.0	794.2	7.12E+06	1	22183.8	22183.8
CO2_54	19727	868.2	508.1	6.92E+06	1	7734.8	7734.8
CO2_60	19727	868.2	335.5	6.69E+06	1	-1225.4	-1225.4
CO2_61	12908	568.1	331.6	6.69E+06	1	-1489.0	-1489.0
CO2_62	7228	318.1	335.5	6.69E+06	1	-1225.4	-1225.4
CO2_Cmix	12499	550.1	335.5	6.69E+06	1	-1225.4	-1225.4
CO2_Hmix	19727	868.2	492.1	2.95E+07	0	4084.0	4084.0
CO2_SPTA	17645	776.6	973.2	2.74E+07	0	31426.3	31426.3
CO2_Tmix	17645	776.6	795.9	7.12E+06	1	22272.7	22272.7

IDAES sCO2 Model Differences



	IDAES		Aspen Difference		EPS Difference	
	Mass Flow (kg/s)	T (K)	Mass Flow (kg/s)	T (K)	Mass Flow (kg/s)	T (K)
CO2_10	568.1	294.9	10.7	0.0	0.1	0.0
CO2_20	568.1	323.2	10.7	0.0	0.1	-0.2
CO2_21	318.1	478.6	0.0	3.6	0.0	3.7
CO2_22_Seal_in	18.0	323.2	10.6	0.0	0.0	-0.2
CO2_22_Seal_out	18.0	299.9				
CO2_23	550.1	323.2	0.1	0.0	0.1	-0.2
CO2_30	550.1	500.2	0.1	13.0	0.1	12.9
CO2_31	789.9	492.1	0.1	9.5	0.0	9.5
CO2_32	789.9	771.4	0.1	-2.7	0.0	-2.7
CO2_33	78.3	492.1	0.0	9.5	0.0	9.5
CO2_34	78.3	793.2	0.0	0.0	0.0	0.0
CO2_35	868.2	773.3	0.0	-2.5	0.0	-2.5
CO2_40_Enter	868.2	973.2	0.0	0.0	0.0	0.0
CO2_40_Exit	868.2	973.2				
CO2_41	91.6	973.2	-0.1	0.0	-0.1	0.0
CO2_42	159.6	973.2	2.8	0.0	2.8	0.0
CO2_43	617.0	973.2	-2.7	0.0	-2.7	0.0
CO2_50	868.2	796.8	0.0	0.1	0.0	0.2
CO2_51	91.6	804.6	-0.1	0.2	-0.1	0.1
CO2_52	159.6	802.5	2.8	0.0	2.8	0.0
CO2_53	617.0	794.2	-2.7	0.0	-2.7	0.1
CO2_54	868.2	508.1	0.0	14.3	0.0	14.4
CO2_60	868.2	335.5	0.0	1.8	0.0	1.9
CO2_61	568.1	331.6	10.7	-1.8	0.1	2.3
CO2_62	318.1	335.5	0.0	2.4	0.0	2.5
CO2_Cmix	550.1	335.5	0.0	2.4		
CO2_Hmix	868.2	492.1	0.1	9.5		
CO2_SPTA	776.6	973.2	0.1	0.0		
CO2_Tmix	776.6	795.9	0.1	0.0		

IDAES TES Variable Integration Approach



Possible Next Steps

- Update system model to operate in off design conditions
- Tie-in existing TES python script for dynamic heat transfer
  - Python scripts cannot be incorporated directly into Aspen Plus through an existing block
    - Convert existing python script to a format accepted by Aspen Plus: Fortran or Excel
    - Run Aspen Plus through Python and incorporate the TES script outputs as block or stream inputs
- IDAES Power Cycle Integration with TES and Flue Gas System
- Test the IDAES Model with Dynamic Models

QUESTIONS?

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