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ASPEN Plus Simulation of CO_2 Recovery Process

Final Report

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Abstract

ASPEN Plus simulations have been created for a CO_2 capture process based on adsorption by monoethanolamine (MEA). Three separate simulations were developed, one each for the flue gas scrubbing, recovery, and purification sections of the process. Although intended to work together, each simulation can be used and executed independently. The simulations were designed as template simulations to be added as a component to other more complex simulations. Applications involving simple cycle or hybrid power production processes were targeted. The default block parameters were developed based on a feed stream of raw flue gas of approximately 14 volume percent CO_2 with a 90% recovery of the CO_2 as liquid.

This report presents detailed descriptions of the process sections as well as technical documentation for the ASPEN simulations including the design basis, models employed, key assumptions, design parameters, convergence algorithms, and calculated outputs.

Introduction

The purpose of this project was to develop a set of ASPEN Plus simulation templates for CO_2 capture technologies. Analysis and quantification of the "CO_2 capture penalty" is becoming of increasing importance. This includes identification of impacts on conventional fossil fueled power plants, hybrid power production systems, and more extensive life cycle analyses. To facilitate this effort, template simulations will greatly reduce the effort needed to determine the impacts of CO_2 capture and compare the effects across various power production processes.

The simulations were developed at a scope commensurate with prior NETL simulations designed to perform systems analysis. The primary calculated quantities of interest are the component flow rates of the main species and the heat duties and power requirements for the process.

The CO_2 capture and recovery technology employed is solvent absorption using monoethanolamine (MEA). The simulations were designed to make it relatively simple to replace the MEA components with the primary species encountered in alternate solvent based absorption processes for CO_2 capture.

For the MEA-based capture technology, the predominant species in the system are CO_2, MEA, and water. Other important species are the contaminants to be removed from the flue gas and some of the ionic species that are formed in solution.

The simulations are intended to be templates that can be inserted into other ASPEN simulations. The report presents the overall process inputs and outputs that must be accounted for when any of the templates is inserted into an existing ASPEN simulation.

The simulations were also designed to be used on a stand-alone basis. Further, they were designed to allow at least limited studies and analysis by users not familiar with the ASPEN Plus software. For each simulation, an Excel user interface was developed to assist the user in setting inputs, launching the simulation engine, and viewing results.

Overall Process Description

The process is designed to capture CO_2 from flue gas and to recover “food grade” carbon dioxide. The process has been broken down into three separate sections: a flue gas scrubbing section, a CO_2 recovery section, and a CO_2 purification and liquefaction section.

Template simulations have been created for each section. Each can operate on a standalone basis or in combination with any or all of the others.

The feed stream to the overall process is a portion of the flue gas from a coal-fired boiler. The main impurities to be removed for production of food grade carbon dioxide are sulfur dioxide, halides, oxides of nitrogen, and particulates, including any trace elements. Carbon dioxide further must be separated from other noncondensible gases (nitrogen, argon, oxygen, carbon monoxide), from moisture, and from any hydrocarbons, prior to storage and shipping.

The process for recovery of carbon dioxide from flue gases employs monoethanolamine (MEA) as the solvent. Other acid gases present in the flue gases (SO_2, SO_3, HCI, HF, NO and NO_2), and fly ash (particulates) result in high amine losses (predominantly through the formation of aqueous acids that react with MEA to form amine salts that cannot be regenerated through the steam stripping process). It is preferable to remove these from the gas stream prior to the carbon dioxide recovery step. This is performed in the flue gas scrubbing section.

In the Scrubbing Section, the hot raw flue gas is fed to a blower that raises the gas stream pressure to 17.4 psia for handling through the process equipment. The flue gas then enters the primary gas quenching and scrubber unit for removal of oxides of sulfur, hydrochloric and hydrofluoric acids, and a part of the oxides of nitrogen. The flue gas blower delivers the flue gases to the quenching section, which is followed by two-stage scrubbing. The active component of the scrubbing solution is sodium sulfite, which reacts with sulfur dioxide to form bisulfite. The resulting bisulfite is converted back to sulfite, with make-up caustic soda, prior to recirculation to the scrubber. Build-up of dissolved solids in the scrubbing solution is controlled by a continuous purge from the first stage. The waste liquor contains particulates, sulfate, sulfite, bisulfite and halides of sodium. The liquor is slightly acidic or neutral and may be treated for disposal as such.

The scrubbed gas passes through a final indirect cooler to minimize both the water input to the carbon dioxide recovery unit as well the possibility for formation of condensation mists by the atmospheric vent flue gas.

In the CO_2 Recovery section, CO_2 is absorbed in a solvent (MEA) countercurrently in a packed column. Inerts, oxygen, unabsorbed carbon dioxide, oxides of nitrogen, and hydrocarbons (methane) are scrubbed by a circulating water wash, in a packed section that is installed on top of the absorption section, and vented to the atmosphere from the top of the packed column. The rich solvent solution from the bottom of the absorber is heat exchanged and stripped in a trayed column to obtain carbon dioxide. The stripping vapor is provided by a steam-heated reboiler.

In the Purification Section, the stripped carbon dioxide from the top of the column is cooled, compressed and purified. The final product is liquid carbon dioxide, stored in insulated storage tanks under pressure.

Reference Design Basis

The design basis for the reference case processes a flue gas feed stream with 14.5 volume percent CO_2. The detailed stream composition is provided in Table 1. The feed rate is 87,069 lb/hr (70,400 SCFD) and the net process yield is approximately 200 ton/day of liquid carbon dioxide product at a purity of 99.9%.

ASPEN Simulation Model Defaults

The ASPEN Simulation Model Defaults are provided in Appendix A.

Flue Gas Scrubbing Section

The process flow diagram for the flue gas scrubbing section is shown in Figure 1. The calculated stream data is provided in Tables 1 and 2.

The flue gas feed stream is assumed to be taken from the bottom of the stack and as such has only a small positive pressure that is not high enough to pass through the scrubber, cooler, and carbon dioxide absorber. Hence, compression of the flue gas is required. The flue gas pressure is boosted to a design pressure of approximately 3 psig so that it will pass through the system. The blower (B-101) is modeled using the isentropic efficiency method. An isentropic efficiency of 0.61 was used. This was determined iteratively by adjusting the efficiency until the unit's exit gas temperature matched the value from an existing commercial process operating under similar conditions.

The flue gas blower exhaust is introduced to a quench section that is followed by two-stage scrubbing in a horizontal spray-baffle scrubber. The quench section saturates the incoming gas stream prior to its introduction to the scrubber vessel. This section is equipped with a pressure control damper which maintains constant inlet pressure to the scrubber. The scrubbing liquid used in this stage is fed to a common manifold that feeds the quench section and the first stage of scrubbing. Flue gases traverse baffles and a Chevron type mist eliminator to enter the second stage of scrubbing. In the second stage of the scrubber, more baffles are encountered. The scrubbing liquid is introduced at an approximate pH of 7.1. A liquid level controller is used to control blowdown from this stage to the first. Each stage has separate pH controllers for addition of caustic soda. The water used in spray washing the mist eliminators serves as makeup too.

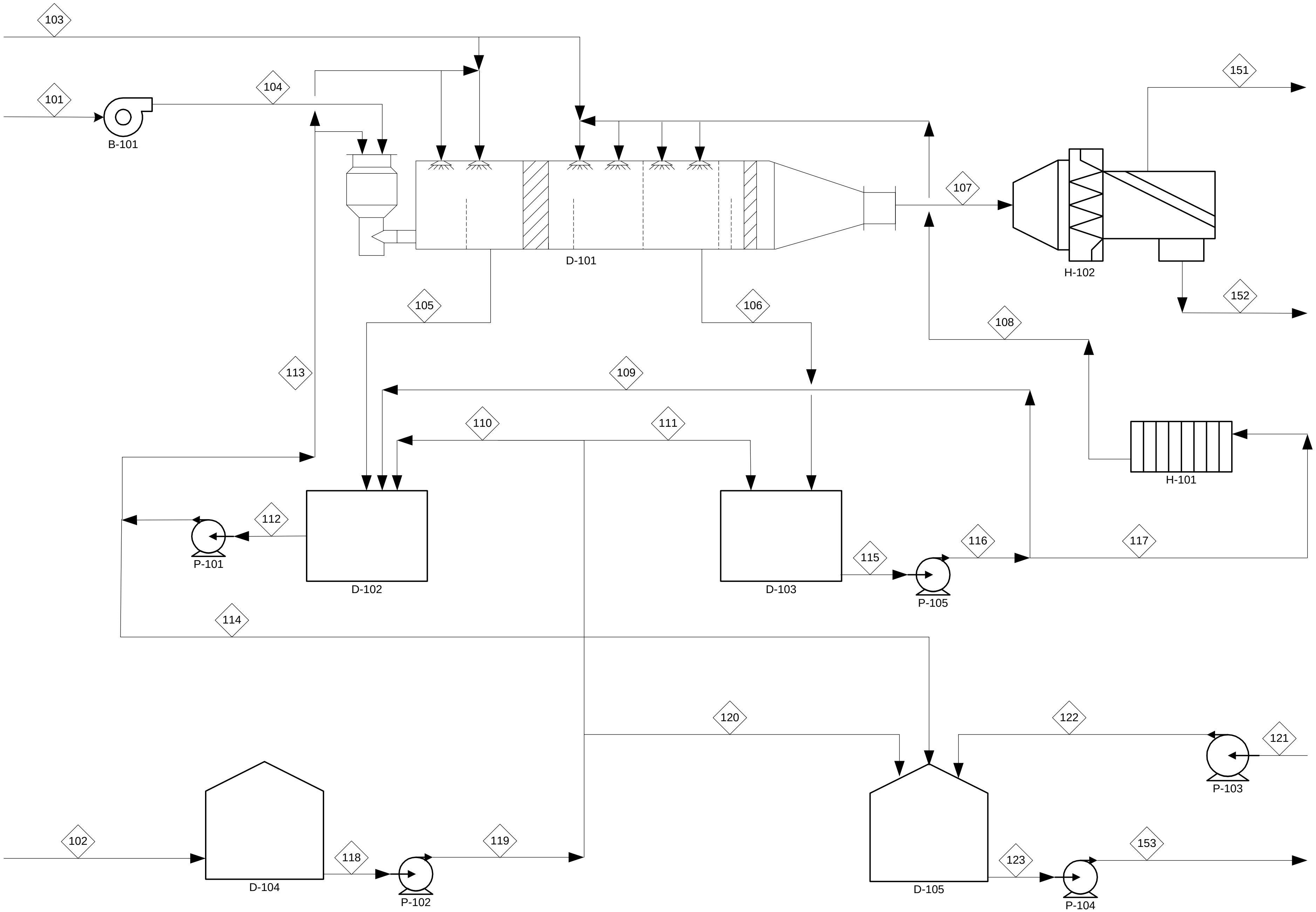

Figure 1 Flue Gas Scrubbing Section

Table 1 Stream Table - Flue Gas Scrubbing Section - Mass Flows

	#101	#102	#103	#104	#105	#106	#107	#108	#109	#110	#111	#112	#113
Temperature F	265	77	77	346.5	139	129.3	129.3	125.6	128.6	77	77	137.5	137.6
Pressure psi	13.5	24.7	20	17.4	17.2	17	17	22	22	29.7	29.7	17.2	21.2
Vapor Frac	1	0	0	1	0	0	1	0	0	0	0	0	0
Mole Flow lbmol/hr	2930.086	370.056	222.034	2930.086	12570.77	16224.18	3109.258	16034.26	428.019	185.028	184.991	13239.32	12828.85
Mass Flow lb/hr	87069.33	6666.667	4000	87069.33	227182.1	293680.8	90273.83	290223	7747.225	3333.333	3332.667	239262.7	231844.5
Volume Flow cuft/hr	1.69E+06	107.09	64.255	1.46E+06	3791.383	4821.213	1.15E+06	4758.963	127.136	53.544	53.534	3987.749	3864.072
Enthalpy MMBtu/hr	-91.01	-45.502	-27.301	-89.198	-1531.664	-1981.321	-112.54	-1959.19	-52.275	-22.751	-22.746	-1613.515	-1563.485
Mass Flow lb/hr													
H2O	3984	6666.667	4000	3984	225710.7	291168.1	7236.151	287775.6	7681.894	3333.333	3332.667	237725.9	230355.3
MEA													
H2S													
CO2	18720			18720	1113.057	2112.131	18683.77	2057.199	54.915			1167.972	1131.765
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	3074.667			3074.667	29.512	43.751	3073.717	42.614	1.138			30.65	29.7
N2	61244			61244	233.957	342.913	61236.47	334.006	8.916			242.873	235.343
AR													
CO	14.667			14.667	0.064	0.094	14.665	0.091	0.002			0.066	0.064
HSS													
H3N													
PARTIC	2.667			2.667	86.021							86.021	83.354
NO2	9.333			9.333	8.045	12.697	9.074	12.367	0.33			8.375	8.115
NAOH					< 0.001							< 0.001	< 0.001
SO2	20			20	0.754	1.145	19.976	1.115	0.03			0.784	0.76
NA+													
HSO3-													
SO3-2													
NANO3					0.002	0.001	trace	0.001	< 0.001			0.002	0.002
NANO2					0.005							0.005	0.005
H2SO3					0.029							0.029	0.029
NAHSO3					0.021							0.021	0.021

Table 1 Stream Table - Flue Gas Scrubbing Section - Mass Flows

	#114	#115	#116	#117	#118	#119	#120	#121	#122	#123	#131	#132	#133
Temperature F	137.6	128.5	128.6	128.6	77	77	77	77	77	135.5	139	137.6	132.1
Pressure psi	21.2	17	22	22	24.7	29.7	29.7	20	24.2	21.2	17.2	21.2	17.2
Vapor Frac	0	0	0	0	0	0	0	0	0	0	1	0	0.163
Mole Flow lbmol/hr	410.419	16462.28	16462.28	16034.26	370.056	370.056	0.037	14.802	14.802	425.258	3243.671	13239.32	19333.44
Mass Flow lb/hr	7417.143	297970.2	297970.2	290223	6666.667	6666.667	0.667	266.667	266.667	7684.477	92731.65	239262.7	383954.6
Volume Flow cuft/hr	123.619	4889.911	4889.848	4762.712	107.09	107.089	0.011	4.284	4.284	127.893	1.21E+06	3987.71	1.16E+06
Enthalpy MMBtu/hr	-50.019	-2010.597	-2010.591	-1958.316	-45.502	-45.502	-0.005	-1.82	-1.82	-51.843	-126.279	-1613.511	-2092.295
Mass Flow lb/hr													
H2O	7369.503	295457.5	295457.5	287775.6	6666.667	6666.667	0.667	266.667	266.667	7636.836	9628.639	237725.9	298404.2
MEA													
H2S													
CO2	36.207	2112.114	2112.114	2057.199						36.207	18738.71	1167.972	20795.9
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	0.95	43.752	43.752	42.614						0.95	3074.854	30.65	3117.468
N2	7.529	342.922	342.922	334.006						7.529	61245.38	242.873	61579.39
AR													
CO	0.002	0.094	0.094	0.091						0.002	14.667	0.066	14.759
HSS													
H3N													
PARTIC	2.667									2.667		86.021	
NO2	0.26	12.697	12.697	12.367						0.26	9.404	8.375	21.771
NAOH	trace									trace		< 0.001	
SO2	0.024	1.145	1.145	1.115						0.024	20.005	0.784	21.12
NA+													
HSO3-													
SO3-2													
NANO3	< 0.001	0.001	0.001	0.001						< 0.001	< 0.001	0.002	0.001
NANO2	< 0.001									< 0.001		0.005	
H2SO3	0.001									0.001		0.029	
NAHSO3	0.001									0.001		0.021	

Table 1   Stream Table - Flue Gas Scrubbing Section - Mass Flows

	#134	#135	#136	#137	#138	#139	#140	#141	#142	#143	#144	#145	#151
Temperature F	136.5	77	77	77	77	108	60	60	114.3	60	60	113.6	108
Pressure psi	17.4	20	20	20	20	17	14.7	19.7	14.7	14.7	19.7	14.7	17
Vapor Frac	0.202	0	0	0	0	0.937	0	0	0	0	0	0	1
Mole Flow lbmol/hr	15814.44	55.508	55.508	53.288	55.508	3109.258	4459.415	4459.415	4459.415	953.962	953.962	953.962	2912.919
Mass Flow lb/hr	319913.8	1000	1000	960	1000	90273.83	80337.62	80337.62	80337.62	17185.89	17185.89	17185.89	86697
Volume Flow cuft/hr	1.18E+06	16.064	16.064	15.421	16.064	1.04E+06	1287.997	1287.978	1299.927	275.529	275.526	278.033	1.04E+06
Enthalpy MMBtu/hr	-1659.508	-6.825	-6.825	-6.552	-6.825	-116.685	-549.695	-549.693	-545.34	-117.591	-117.591	-116.672	-92.578
Mass Flow lb/hr													
H2O	235339.3	1000	1000	960	1000	7236.151	80337.62	80337.62	80337.62	17185.89	17185.89	17185.89	3728.927
MEA													
H2S													
CO2	19851.77					18683.77							18620.68
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	3104.366					3073.717							3072.997
N2	61479.34					61236.47							61230.96
AR													
CO	14.731					14.665							14.663
HSS													
H3N													
PARTIC	86.021												
NO2	17.448					9.074							8.816
NAOH	< 0.001												
SO2	20.76					19.976							19.956
NA+													
HSO3-													
SO3-2													
NANO3	0.002					trace							trace
NANO2	0.005												
H2SO3	0.029												
NAHSO3	0.021												

Table 1 Stream Table - Flue Gas Scrubbing Section - Mass Flows

	#152	#153	#154
Temperature F	108	135.5	77
Pressure psi	17	24.2	20
Vapor Frac	0	0	0
Mole Flow lbmol/hr	196.339	425.258	2.22
Mass Flow lb/hr	3576.829	7684.477	40
Volume Flow cuft/hr	59.139	127.893	0.643
Enthalpy MMBtu/hr	-24.107	-51.843	-0.273
Mass Flow lb/hr			
H2O	3507.225	7636.836	40
MEA			
H2S			
CO2	63.094	36.207	
HCO3-			
MEACOO-			
MEA+			
CO3-2			
HS-			
S-2			
H3O+			
OH-			
O2	0.721	0.95	
N2	5.51	7.529	
AR			
CO	0.002	0.002	
HSS			
H3N			
PARTIC		2.667	
NO2	0.258	0.26	
NAOH		trace	
SO2	0.02	0.024	
NA+			
HSO3-			
SO3-2			
NANO3	trace	< 0.001	
NANO2		< 0.001	
H2SO3		0.001	
NAHSO3		0.001	

Table 2 Stream Table - Flue Gas Scrubbing Section - Mass Fractions

	#101	#102	#103	#104	#105	#106	#107	#108	#109	#110	#111	#112	#113
Temperature F	265	77	77	346.5	139	129.3	129.3	125.6	128.6	77	77	137.5	137.6
Pressure psi	13.5	24.7	20	17.4	17.2	17	17	22	22	29.7	29.7	17.2	21.2
Vapor Frac	1	0	0	1	0	0	1	0	0	0	0	0	0
Mole Flow lbmol/hr	2930.086	370.056	222.034	2930.086	12570.77	16224.18	3109.258	16034.26	428.019	185.028	184.991	13239.32	12828.85
Mass Flow lb/hr	87069.33	6666.667	4000	87069.33	227182.1	293680.8	90273.83	290223	7747.225	3333.333	3332.667	239262.7	231844.5
Volume Flow cuft/hr	1.69E+06	107.09	64.255	1.46E+06	3791.383	4821.213	1.15E+06	4758.963	127.136	53.544	53.534	3987.749	3864.072
Enthalpy MMBtu/hr	-91.01	-45.502	-27.301	-89.198	-1531.664	-1981.321	-112.54	-1959.19	-52.275	-22.751	-22.746	-1613.515	-1563.485
Mass Frac													
H2O	0.046	1	1	0.046	0.994	0.991	0.08	0.992	0.992	1	1	0.994	0.994
MEA													
H2S													
CO2	0.215			0.215	0.005	0.007	0.207	0.007	0.007			0.005	0.005
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	0.035			0.035	130 PPM	149 PPM	0.034	147 PPM	147 PPM			128 PPM	128 PPM
N2	0.703			0.703	0.001	0.001	0.678	0.001	0.001			0.001	0.001
AR													
CO	168 PPM			168 PPM	280 PPB	320 PPB	162 PPM	315 PPB	315 PPB			276 PPB	276 PPB
HSS													
H3N													
PARTIC	31 PPM			31 PPM	379 PPM							360 PPM	360 PPM
NO2	107 PPM			107 PPM	35 PPM	43 PPM	101 PPM	43 PPM	43 PPM			35 PPM	35 PPM
NAOH					trace							trace	trace
SO2	230 PPM			230 PPM	3 PPM	4 PPM	221 PPM	4 PPM	4 PPM			3 PPM	3 PPM
NA+													
HSO3-													
SO3-2													
NANO3					11 PPB	3 PPB	trace	3 PPB	3 PPB			10 PPB	11 PPB
NANO2					20 PPB							19 PPB	20 PPB
H2SO3					127 PPB							120 PPB	124 PPB
NAHSO3					93 PPB							88 PPB	91 PPB

Table 2 Stream Table - Flue Gas Scrubbing Section - Mass Fractions

	#114	#115	#116	#117	#118	#119	#120	#121	#122	#123	#131	#132	#133
Temperature F	137.6	128.5	128.6	128.6	77	77	77	77	77	135.5	139	137.6	132.1
Pressure psi	21.2	17	22	22	24.7	29.7	29.7	20	24.2	21.2	17.2	21.2	17.2
Vapor Frac	0	0	0	0	0	0	0	0	0	0	1	0	0.163
Mole Flow lbmol/hr	410.419	16462.28	16462.28	16034.26	370.056	370.056	0.037	14.802	14.802	425.258	3243.671	13239.32	19333.44
Mass Flow lb/hr	7417.143	297970.2	297970.2	290223	6666.667	6666.667	0.667	266.667	266.667	7684.477	92731.65	239262.7	383954.6
Volume Flow cuft/hr	123.619	4889.911	4889.848	4762.712	107.09	107.089	0.011	4.284	4.284	127.893	1.21E+06	3987.71	1.16E+06
Enthalpy MMBtu/hr	-50.019	-2010.597	-2010.591	-1958.316	-45.502	-45.502	-0.005	-1.82	-1.82	-51.843	-126.279	-1613.511	-2092.295
Mass Frac													
H2O	0.994	0.992	0.992	0.992	1	1	1	1	1	0.994	0.104	0.994	0.777
MEA													
H2S													
CO2	0.005	0.007	0.007	0.007						0.005	0.202	0.005	0.054
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	128 PPM	147 PPM	147 PPM	147 PPM						124 PPM	0.033	128 PPM	0.008
N2	0.001	0.001	0.001	0.001						980 PPM	0.66	0.001	0.16
AR													
CO	276 PPB	315 PPB	315 PPB	315 PPB						266 PPB	158 PPM	276 PPB	38 PPM
HSS													
H3N													
PARTIC	360 PPM									347 PPM		360 PPM	
NO2	35 PPM	43 PPM	43 PPM	43 PPM						34 PPM	101 PPM	35 PPM	57 PPM
NAOH	trace									trace		trace	
SO2	3 PPM	4 PPM	4 PPM	4 PPM						3 PPM	216 PPM	3 PPM	55 PPM
NA+													
HSO3-													
SO3-2													
NANO3	10 PPB	3 PPB	3 PPB	3 PPB						10 PPB	trace	10 PPB	2 PPB
NANO2	19 PPB									19 PPB		19 PPB	
H2SO3	120 PPB									116 PPB		120 PPB	
NAHSO3	88 PPB									85 PPB		88 PPB	

Table 2 Stream Table - Flue Gas Scrubbing Section - Mass Fractions

	#134	#135	#136	#137	#138	#139	#140	#141	#142	#143	#144	#145	#151
Temperature F	136.5	77	77	77	77	108	60	60	114.3	60	60	113.6	108
Pressure psi	17.4	20	20	20	20	17	14.7	19.7	14.7	14.7	19.7	14.7	17
Vapor Frac	0.202	0	0	0	0	0.937	0	0	0	0	0	0	1
Mole Flow lbmol/hr	15814.44	55.508	55.508	53.288	55.508	3109.258	4459.415	4459.415	4459.415	953.962	953.962	953.962	2912.919
Mass Flow lb/hr	319913.8	1000	1000	960	1000	90273.83	80337.62	80337.62	80337.62	17185.89	17185.89	17185.89	86697
Volume Flow cuft/hr	1.18E+06	16.064	16.064	15.421	16.064	1.04E+06	1287.997	1287.978	1299.927	275.529	275.526	278.033	1.04E+06
Enthalpy MMBtu/hr	-1659.508	-6.825	-6.825	-6.552	-6.825	-116.685	-549.695	-549.693	-545.34	-117.591	-117.591	-116.672	-92.578
Mass Frac													
H2O	0.736	1	1	1	1	0.08	1	1	1	1	1	1	0.043
MEA													
H2S													
CO2	0.062					0.207							0.215
HCO3-													
MEACOO-													
MEA+													
CO3-2													
HS-													
S-2													
H3O+													
OH-													
O2	0.01					0.034							0.035
N2	0.192					0.678							0.706
AR													
CO	46 PPM					162 PPM							169 PPM
HSS													
H3N													
PARTIC	269 PPM												
NO2	55 PPM					101 PPM							102 PPM
NAOH	trace												
SO2	65 PPM					221 PPM							230 PPM
NA+													
HSO3-													
SO3-2													
NANO3	8 PPB					trace							trace
NANO2	15 PPB												
H2SO3	90 PPB												
NAHSO3	66 PPB												

Table 2 Stream Table - Flue Gas Scrubbing Section - Mass Fractions

	#152	#153	#154
Temperature F	108	135.5	77
Pressure psi	17	24.2	20
Vapor Frac	0	0	0
Mole Flow lbmol/hr	196.339	425.258	2.22
Mass Flow lb/hr	3576.829	7684.477	40
Volume Flow cuft/hr	59.139	127.893	0.643
Enthalpy MMBtu/hr	-24.107	-51.843	-0.273
Mass Frac			
H2O	0.981	0.994	1
MEA			
H2S			
CO2	0.018	0.005	
HCO3-			
MEACOO-			
MEA+			
CO3-2			
HS-			
S-2			
H3O+			
OH-			
O2	201 PPM	124 PPM	
N2	0.002	980 PPM	
AR			
CO	429 PPB	266 PPB	
HSS			
H3N			
PARTIC		347 PPM	
NO2	72 PPM	34 PPM	
NAOH		trace	
SO2	6 PPM	3 PPM	
NA+			
HSO3-			
SO3-2			
NANO3	1 PPB	10 PPB	
NANO2		19 PPB	
H2SO3		116 PPB	
NAHSO3		85 PPB	

The scrubber is modeled as a two-stage equilibrium flash, operating in series. The scrubbing solution is split and fed into both stages. The split is approximately 44% to stage 1 and 56% to stage 2. The overall unit operates adiabatically. The heat given off in the quench section of stage one is used as input to stage two. The gas temperature exiting the first and second stages is about 149 °F and 131 °F, respectively. The temperature at the second stage outlet is controlled by the degree of cooling of the scrubbing liquid introduced, so as to maintain water balance in the system.

The reactions involved in the scrubbing process are as follows:

$$SO_2 + H_2O \longleftrightarrow H_2SO_3$$
$$SO_2 + NaOH \longleftrightarrow NaHSO_3$$
$$SO_2 + 2NaOH \longleftrightarrow Na_2SO_3 + H_2O$$
$$SO_2 + H_2O + Na_2SO_3 \longleftrightarrow 2NaHSO_3$$
$$2Na_2SO_3 + O_2 \longleftrightarrow 2Na_2SO_4$$

In the process, sodium sulfite is deemed as the active component and is regenerated by fresh caustic in the recirculation tank. Of the acid gases other than SO_2, the hydrochloric and hydrofluoric acids react with the hydroxide, producing the respective halides.
Oxides of nitrogen present in the flue gases are likely to be nitrogen dioxide and nitric oxide. Nitrogen dioxide will form nitrate and nitrite as follows:

$$2NaOH + 2NO_2 \longleftrightarrow NaNO_3 + NaNO_2 + H_2O$$

The sulfur dioxide content of the scrubbed gases is targeted to be less than 10 parts per million.

There is a need to maintain a water balance in the flue gas scrubber and in the carbon dioxide recovery unit. At the inlet to the scrubber, the moisture content of the incoming flue gas is dependent on the type of coal, inherent moisture content, and how wet the coal is when fired. Control of the water balance is achieved by control of the temperature of scrubbed flue gases exiting the second stage of scrubbing. For the reference design, this temperature is 131°F. The main factor in the water balance, for the CO_2 Recovery Section is the water content of the CO_2 absorber vent in relation to the scrubbed flue gases entering the carbon dioxide recovery unit. In approximate terms, if the moisture content of the absorber vent and carbon dioxide (to purification) exceeds that of the scrubbed flue gas entering the carbon dioxide recovery unit, the concentration of MEA in the circulating solvent will increase, and makeup water must be added to maintain the desired concentration. If the amount of moisture in the scrubbed flue gas exceeds that contained in the absorber vent and carbon dioxide (to purification), the MEA concentration will decrease, and reflux water from the stripper must be discarded to control the MEA concentration of the circulating solvent. Neither situation is desirable. The makeup water is condensate, which has a cost associated with it. On the other hand, disposal of reflux water, which contains about one-half of one percent MEA, is expensive too, not only for the cost of make-up chemical but also for the cost of treatment.
Hence, the need for adjustment of the moisture content of the scrubbed flue gas entering the carbon dioxide recovery unit is met by condensing the water that would have otherwise constituted surplus reflux water. Although the moisture content of the flue gases varies with

coal type and season, a cooling temperature of 108°F will produce minimal levels of both makeup and effluent.

The cooler provided to condense the excess water is of a bare tube design, with process water on the tube side and a temperature control of the water flow. The cooler condensed water is pumped to the cooling water return line.
The cooler is also modeled as an equilibrium flash operation. A calculator block is used to determine the flow of water required to perform the necessary cooling. A 15 °F hot-side temperature approach is assumed.

The solute rich solution from each stage is collected and recycled back to the respective scrubbing stage. The first stage solution recycle undergoes a straining step to remove undissolved solids. The second stage recycle passes through a cooler to remove the heat of solution and some sensible heat taken up from the flue gas. As with the final gas cooler, this unit is cooled by process water. A second calculator block is used to determine the flow of water required to perform the necessary cooling. A 15 °F hot-side temperature approach is assumed. A small blowdown stream from stage two is fed to the stage one collection drum, connecting the two recycle loops.

The strainer is modeled as a simple separator block assumed to operate at 100% efficiency in removing particulates.

The inputs to the process are: the flue gas feed conditions (composition, temperature, and pressure), the desired flue gas exit temperature, and the spent solution flow as a percentage of the inlet flue gas flow rate. The calculated quantities are exit stream flows and conditions (cleaned flue gas, condensate from gas cooler, and spent solution), the makeup solution amounts, the duties for the flue gas blower and solution pumps, and the cooling water requirements.

<u>ASPEN Unit Operations Blocks</u>
Following is a description of each ASPEN Unit Operations Block in the simulation.

B-101 – Inlet flue gas blower
Compr Block, Discharge pressure 17.4 psia, Isentropic efficiency 0.61, Mechanical efficiency 0.97

D-101A – Flue gas scrubber stage 1
Flash2 Block, Temperature 139 °F, Pressure 17.2 psia

D-101B – Flue gas scrubber stage 2
Flash2 Block, Pressure 17.0 psia, adiabatic mode with inlet heat stream as the outlet heat stream from D-101A

D-102 – Stage 1 solvent holdup tank
Mixer Block, Adiabatic, 0 pressure drop

D-103 – Stage 2 solvent holdup tank
Mixer Block, Adiabatic, 0 pressure drop

D-104 – Inlet makeup solution holdup tank
Mixer Block, Adiabatic, 0 pressure drop

D-105 – Waste solvent solution holdup tank
Mixer Block, Adiabatic, 0 pressure drop

H-101 – Stage 2 recycle solvent cooler, solvent side
Heater Block, Temperature change -3 °F, pressure drop 4 psia

H-101B – Stage 2 recycle solvent cooler, process water side
Heater Block, Adiabatic operation with inlet heat stream from Block H-101 outlet stream with 5% heat loss imposed, pressure drop 5 psia

H-102 – Final flue gas cooler, gas side
Heater Block, Temperature 108 °F, pressure drop 0.4 psia

H-102B – Final flue gas cooler, process water side
Heater Block, Adiabatic operation with inlet heat stream from Block H-102 outlet stream with 5% heat loss imposed, pressure drop 5 psia

M-101 – Stage 1 solvent mixer block to holdup tank
Mixer Block, Adiabatic, 0 pressure drop

M-102 – Stage 2 solvent mixer block to holdup tank
Mixer Block, Adiabatic, 0 pressure drop

M-103 – Makeup water stream splitter
Fsplit Block, Split fractions 0.25 for #135, 0.25 for #136, 0.24 for #137, 0.25 for #138, 0.01 for #154

M-104 – Stage 1 solvent recycle splitter from holdup tank
Fsplit Block, Split fractions 0.969 for 113, 0.031 for #114

M-105 – Makeup solvent spltter
Fsplit Block, Split fractions 0.5 for 110, 0.4999 for #111, 0.0001 for #120

M-106 – Stage 2 solvent recycle splitter from holdup tank
Fsplit Block, Split fractions 0.026 for #109, 0.974 for #117

M-107 – Specialty ASPEN Block to set heat duty to water side of solvent cooler
Mult Block, Factor 1.05

M-108 – Specialty ASPEN Block to set heat duty to water side of final flue gas cooler
Mult Block, Factor 1.05

P-101 – Stage 1 solvent recycle pump
Pump Block, Pressure increase 4 psia, Driver efficiency 0.97

P-102 – Makeup solvent feed pump
Pump Block, Pressure increase 5 psia, Driver efficiency 0.97

P-103 – Makeup caustic feed pump
Pump Block, Discharge pressure increase 24.2 psia, Driver efficiency 0.97

P-104 – Waste solvent exit pump
Pump Block, Pressure increase 3 psia, Driver efficiency 0.97

P-105 – Stage 2 solvent recycle pump
Pump Block, Pressure increase 5 psia, Driver efficiency 0.97

P-106 – Cooling water pump for H101B
Pump Block, Pressure increase 5 psia, Driver efficiency 0.97

P-107 – Cooling water pump for H102B
Pump Block, Pressure increase 5 psia, Driver efficiency 0.97

S-101 – Final flue gas cooler vapor/liquid separator
Flash2 Block, Adiabatic operation, 0 pressure drop

ASPEN Auxiliary Blocks

CW-1 and CW-2 are calculator blocks that set the cooling water flow rate for H-101 and H-102 respectively to achieve a hot-side temperature approach of 15 °F.

Simulation Convergence

Convergence of the ASPEN simulation is accomplished through two nested Convergence Blocks, both employing the bounded Wegstein method with relative tolerances of 0.0001. The outer loop contains the solvent recycle to stage 1, stream #113, as the tear stream and is converged with the block RSOLSTA1. The inner loop contains the solvent recycle to stage 2, stream #115, as the tear stream and is converged with the block RSOLSTA2.

The calculation sequence is:

P-103, D-104, P-102, M-105, M-103, B-101

→ Convergence Block RSOLSTA1

M-101 D-101A

→ Convergence Block RSOLSTA2

P-105, M-106, H-101, M-102, D-101B, D-103

D-102, P-101, M-104

S-101, D-105, P-104

CO_2 Recovery Section

The input to the CO_2 Recovery section is assumed to be a wet, scrubbed (particulate free) flue gas at a temperature of approximately 108°F. The process flow diagram is shown in Figure 2. The calculated stream data is provided in Tables 3 and 4. As with the scrubbing section, the ELECNRTL physical property option set was selected. This was done to enable more accurate predictions of ionization equilibrium and the heats of solution.

The flue gas stream is fed into the bottom of the MEA absorber. The absorber MEA solution is fed at the top of the column and flows countercurrent to the flue gas. The solvent solution enters at 104°F and heats up gradually with the progress of absorption. The CO_2 rich solvent solution attains a temperature of 133°F at the bottom of the absorber.

The absorber is modeled in ASPEN using RadFrac, a rigorous, "plate-to-plate" equilibrium stage model that allows for chemical reactions as well as phase equilibrium at each stage. The following set of chemical reactions were enabled within the absorber column:

$$MEA^+ + H_2O \longleftrightarrow MEA + H_3O^+$$
$$CO_2 + OH^- \longleftrightarrow HCO_3^-$$
$$HCO_3^- + H_2O \longleftrightarrow H_3O^+ + CO_3^{-2}$$
$$MEACOO^- + H_2O \longleftrightarrow MEA + HCO_3^-$$
$$2\,H_2O \longleftrightarrow H_3O^+ + OH\text{-}$$
$$H_2O + H_2S \longleftrightarrow HS^- + H_3O^+$$
$$H_2O + HS^- \longleftrightarrow S^{-2} + H_3O^+$$

At the operating conditions, experimental data suggests that reaction 2 is too slow to reach chemical equilibrium. Therefore a temperature approach to equilibrium of 46 °F was specified. Using this value the calculated outlet streams agreed with operating data from another source. The solvent feed for the absorber is the bottoms stream from the stripper column. The absorber is modeled using 10 equilibrium stages and a condenser pressure set at 14.5 psia.

The absorber is equipped with a water wash section to reduce amine losses in the absorber vent. This packed section has a draw-off tray to cool the circulating water.
One physical phenomenon to be guarded against is the formation of condensation mist consisting of fine particles of MEA. This will occur if there is a rapid cooling of the inlet gas as it moves up to the top of the absorber, all the more if the inlet gas is unsaturated. It is expected that condensation mist will not form, for there is little cooling of the inlet gas before it goes to the absorber vent. The absorber vent contains essentially all the gases in the inlet gas other than 90% of the carbon dioxide that is absorbed. Very small amounts of other gases absorbed along with carbon dioxide are separated in the purification section.

Figure 2 CO_2 Recovery Section

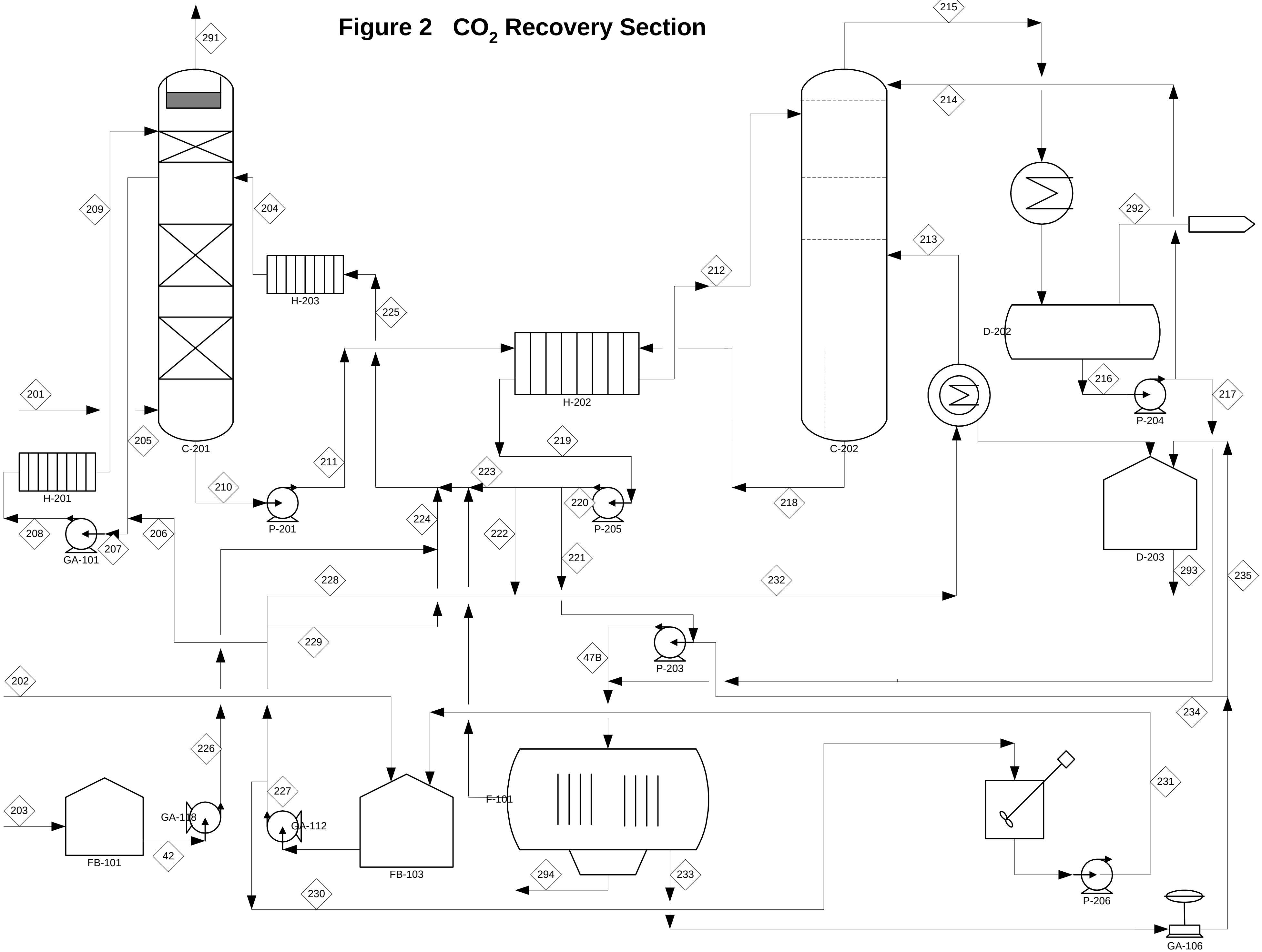

Table 3 Stream Table - CO2 Recovery Section - Mass Flows

	#201	#202	#203	#204	#204R	#205	#206	#207	#208	#209	#210	#211	#212
Temperature F	109	120	75	104	104	108	115.2	113.6	113.6	103	122.8	122.8	205
Pressure psi	16.9	135	20	16.8	16.8	14.5	71.2	14.5	16.5	16.5	16.5	35	35
Vapor Frac	0.999	0	0	0	0	0	0	0	0	0	0	0	0.007
Mole Flow lbmol/hr	2926.442	162.529	0.388	20212.43	20234.85	66411.55	154.038	66565.87	66565.87	66565.16	20388.4	20388.4	20472.12
Mass Flow lb/hr	86980	2928	17.333	417511.3	417761.5	1.20E+06	2777.42	1.20E+06	1.20E+06	1.20E+06	434149.1	434149.1	434149.1
Volume Flow cuft/hr	1.05E+06	47.426	0.271	6.79E+03	6798.54	19657.04	4.50E+01	19412.4	19412.29	19365.38	7202.798	7202.557	35776.93
Enthalpy MMBtu/hr	-94.069	-19.858	-0.046	-2507.879	-2510.509	-8123.753	-18.838	-8142.591	-8142.582	-8155.253	-2582.308	-2582.275	-2547.56
Mass Flow lb/hr													
H2O	3936	2928	2.667	345059.9	345516.4	1.20E+06	2773.696	1.20E+06	1.20E+06	1.20E+06	346565	346564.5	346625.1
MEA			14.667	40414.66	40320.79	15.718	0.003	42.324	42.325	36.619	8105.038	8106.897	18234.84
H2S											trace		
CO2	18705.33			0.202	0.202	9.058	1.618	22.905	22.906	18.954	39.898	39.969	3724.389
HCO3-	< 0.001			377.534	377.257	451.413	0.892	444.572	444.571	449.794	4945.337	4947	4847.809
MEACOO-				18399.17	18332.19	20.78	< 0.001	7.204	7.204	7.287	41874.96	41872.15	33509.13
MEA+			< 0.001	11455.89	11415.96	477.299	0.908	459.265	459.264	465.014	30292.92	30292.71	24987.02
CO3-2				44.726	44.869	2.332	< 0.001	1.09	1.09	1.295	135.647	135.537	30.967
HS-											trace		
S-2											trace		
H3O+	< 0.001	< 0.001		trace	trace	< 0.001	< 0.001	0.001	0.001	0.001	< 0.001	< 0.001	< 0.001
OH-	trace	< 0.001	trace	0.978	0.982	0.204	trace	0.094	0.094	0.084	0.161	0.161	0.271
O2	3074.667			0.002	0.002		0.044	0.044	0.044	0.044	49.153	49.153	49.153
N2	61240			0.004	0.004		0.131	0.131	0.131	0.131	382.472	382.472	382.472
AR	9.333			trace	trace		< 0.001	< 0.001	< 0.001	< 0.001	0.159	0.159	0.159
CO	14.667			trace	trace		< 0.001	< 0.001	< 0.001	< 0.001	0.105	0.105	0.105
HSS				1758.244	1752.879	74.307	0.129	74.436	74.436	74.436	1758.23	1758.23	1758.23
H3N													
PARTIC													
NO2													
NAOH													
SO2	< 0.001			< 0.001	< 0.001		trace	trace	trace	trace	< 0.001	< 0.001	< 0.001
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 3 Stream Table - CO2 Recovery Section - Mass Flows

	#213	#214	#215	#216	#217	#218	#219	#220	#221	#222	#223	#224	#225
Temperature F	318.4	105.2	201.1	105	105.2	239.6	126.3	126.3	126.3	126.3	126.3	114.5	126.4
Pressure psi	58.7	46.2	25.7	26.2	46.2	28.7	28.7	58.7	58.7	58.7	58.7	25	25
Vapor Frac	1	0	1	0	0	0	0	0	0	0	0	0	0
Mole Flow lbmol/hr	34.691	144.425	562.768	230.358	85.924	20308.06	20306.67	20306.67	56.859	20.307	20229.51	5.356	20234.86
Mass Flow lb/hr	667.435	2608.339	18178.89	4160.293	1551.789	419247.8	419247.8	419247.8	1173.894	419.248	417654.6	106.929	417761.5
Volume Flow cuft/hr	4834.157	42.213	154072.9	67.33	25.114	7189.247	6866.097	6865.716	19.224	6.866	6.84E+03	1.728	6.84E+03
Enthalpy MMBtu/hr	-3.541	-17.697	-76.154	-28.227	-10.528	-2467.643	-2511.037	-2510.986	-7.031	-2.511	-2501.444	-0.654	-2502.098
Mass Flow lb/hr													
H2O	605.84	2598.241	4402.529	4144.186	1545.781	346396.5	346707.8	346707.7	970.782	346.708	345390.2	92.145	345482.2
MEA	51.754	0.004	3.874	0.007	0.003	41843.45	40589.46	40589.87	113.652	40.59	40435.63	14.483	40450.58
H2S			trace			trace							
CO2	8.285	4.385	13339.55	6.994	2.609	61.479	0.578	0.579	0.002	0.001	0.577	trace	0.579
HCO3-		2.419		3.859	1.439	1589.367	506.718	507.128	1.42	0.507	505.201	0.003	505.657
MEACOO-		0.002		0.003	0.001	16259.44	18203.8	18203.16	50.969	18.203	18133.99	0.164	18133.42
MEA+		2.463		3.929	1.465	11331.31	11446.06	11446.02	32.049	11.446	11402.52	0.118	11402.6
CO3-2		< 0.001		< 0.001	< 0.001	6.094	32.863	32.826	0.092	0.033	32.701	0.002	32.678
HS-						trace							
S-2						trace							
H3O+		< 0.001		< 0.001	< 0.001	< 0.001	trace	trace	trace	trace	trace	trace	trace
OH-		trace		trace	trace	0.616	0.927	0.927	0.003	0.001	0.924	0.004	0.924
O2	0.004	0.119	49.276	0.19	0.071	< 0.001	< 0.001	< 0.001	trace	trace	< 0.001	0.001	0.002
N2	0.013	0.355	382.839	0.566	0.211	< 0.001	< 0.001	< 0.001	trace	trace	< 0.001	0.004	0.004
AR	< 0.001	< 0.001	0.159	0.001	< 0.001	trace	trace	trace	trace	trace	trace	trace	trace
CO	trace	< 0.001	0.105	< 0.001	< 0.001	trace	trace	trace	trace	trace	trace	trace	trace
HSS	1.539	0.349	0.557	0.557	0.208	1759.561	1759.561	1759.561	4.927	1.76	1752.875	0.004	1752.879
H3N													
PARTIC													
NO2													
NAOH													
SO2	trace	trace	< 0.001	trace	trace	< 0.001	< 0.001	< 0.001	trace	trace	< 0.001	trace	< 0.001
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 3 Stream Table - CO2 Recovery Section - Mass Flows

	#226	#227	#228	#229	#230	#231	#232	#233	#234	#235	#251	#252	#253
Temperature F	75.1	115.2	115.2	115.2	115.2	115.3	122	120.6	120.6	120.6	103	108	108
Pressure psi	25	71.2	71.2	71.2	71.2	81.2	58.7	68.7	68.7	68.7	16.5	14.5	14.5
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	1	1
Mole Flow lbmol/hr	0.388	248.452	14.907	4.969	74.536	74.536	35.21	427.225	341.78	85.445	66232.31	2530.317	71.628
Mass Flow lb/hr	17.333	4479.789	268.787	89.596	1343.937	1343.937	688.035	8434.215	6747.372	1686.843	1.19E+06	71050.42	2054.81
Volume Flow cuft/hr	2.71E-01	72.554	4.353	1.451	21.766	2.18E+01	11.212	137.525	110.02	27.505	19268.53	1.06E+06	3.01E+04
Enthalpy MMBtu/hr	-0.046	-30.385	-1.823	-0.608	-9.116	-9.115	-4.334	-52.673	-42.139	-10.535	-8114.466	-42.001	-0.204
Mass Flow lb/hr													
H2O	2.667	4473.781	268.427	89.476	1342.134	1342.134	615.065	7434.28	5947.425	1486.856	1.19E+06	3818.543	
MEA	14.667	0.004	< 0.001	< 0.001	0.001	0.001	40.336	557.852	446.283	111.57	36.373	< 0.001	
H2S													
CO2		2.61	0.157	0.052	0.783	0.783	0.001	0.01	0.008	0.002	18.839	5322.862	56.863
HCO3-		1.439	0.086	0.029	0.432	0.432	0.777	9.741	7.793	1.948	446.903		
MEACOO-		0.001	< 0.001	< 0.001	< 0.001	< 0.001	18.18	262.362	209.888	52.472	7.228		
MEA+	< 0.001	1.464	0.088	0.029	0.439	0.439	11.806	168.538	134.83	33.708	462.017		
CO3-2		< 0.001	trace	trace	< 0.001	< 0.001	0.079	0.985	0.788	0.197	1.286		
HS-													
S-2													
H3O+		< 0.001	trace	trace	< 0.001	< 0.001	trace	trace	trace	trace	0.001		
OH-	trace	< 0.001	trace	trace	trace	trace	0.002	0.023	0.019	0.005	0.084		
O2		0.071	0.004	0.001	0.021	0.021	0.004	0.106	0.085	0.021	0.044	2805.676	219.883
N2		0.211	0.013	0.004	0.063	0.063	0.013	0.317	0.253	0.063	0.13	59080.79	1776.874
AR		< 0.001	< 0.001	trace	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	8.477	0.698
CO		< 0.001	trace	trace	< 0.001	< 0.001	trace	< 0.001	< 0.001	< 0.001	< 0.001	14.069	0.492
HSS		0.208	0.012	0.004	0.062	0.062	1.772				73.922	0.001	
H3N													
PARTIC													
NO2													
NAOH													
SO2		trace	trace	trace	trace	trace	trace				trace	< 0.001	< 0.001
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 3   Stream Table - CO2 Recovery Section - Mass Flows

	#254	#255	#256	#257	#258	#259	#260	#261	#291	#292	#293	#294
Temperature F	128.8	103	318.4	115	108	126.4	104	105.2	108	105	77	120.6
Pressure psi	14.5	16.5	58.7	46.2	14.5	68.7	16.5	46.2	14.5	26.2	58.7	68.7
Vapor Frac	1	0	0	0	0	0	0	0	1	1	0	0
Mole Flow lbmol/hr	2781.407	332.826	0.708	248.452	66482.98	56.859	20545.25	230.358	2601.945	332.347	86.153	45.932
Mass Flow lb/hr	76340.13	5999.66	20.601	4479.789	1.20E+06	1173.894	423511	4160.293	73105.23	14018.6	1707.444	830.987
Volume Flow cuft/hr	1.21E+06	96.827	0.378	72.556	19448.48	19.224	6891.491	67.329	1.09E+06	76278.14	27.557	13.464
Enthalpy MMBtu/hr	-60.416	-40.776	-0.082	-30.386	-8130.71	-7.031	-2548.655	-28.226	-42.205	-52.687	-10.689	-5.611
Mass Flow lb/hr												
H2O	7050.935	5994.4	9.48	4473.781	1.20E+06	970.781	351053.1	4144.186	3818.543	257.204	1496.571	825.998
MEA	2.333	0.183	10.81	0.004	15.999	113.653	40417.33	0.007	< 0.001	trace	121.423	
H2S	trace											
CO2	5379.694	0.095	< 0.001	2.61	56.863	0.002	0.205	6.994	5379.724	13329.77	< 0.001	
HCO3-		2.246	0.003	1.439	476.193	1.422	382.612	3.859			1.004	
MEACOO-		0.036	0.045	0.001	3.136	50.966	18392.38	0.003			53.883	
MEA+		2.322	0.03	1.464	487.538	32.049	11459.75	3.929			33.896	
CO3-2		0.006	trace	< 0.001	0.485	0.092	46.008	< 0.001			0.344	
HS-												
S-2												
H3O+		trace		< 0.001	0.002	trace	trace	< 0.001			trace	trace
OH-		< 0.001	trace	< 0.001	0.034	0.003	1.004	trace			0.005	trace
O2	3025.516	< 0.001	trace	0.071	219.883	trace	0.002	0.19	3025.56	49.086	0.021	
N2	60857.53	0.001	trace	0.211	1776.874	trace	0.005	0.566	60857.66	382.273	0.063	
AR	9.175	trace	trace	< 0.001	0.698	trace	trace	0.001	9.175	0.158	< 0.001	
CO	14.561	trace		< 0.001	0.492		trace	< 0.001	14.561	0.105	< 0.001	
HSS	0.386	0.371	0.233	0.208	74.307	4.927	1758.616	0.557	0.001	< 0.001	0.233	4.989
H3N												
PARTIC												
NO2												
NAOH												
SO2	< 0.001	trace		trace	< 0.001	trace	< 0.001	trace	< 0.001	< 0.001		trace
NA+												
HSO3-												
SO3-2												
NANO3												
NANO2												
H2SO3												
NAHSO3												

Table 4 Stream Table - CO2 Recovery Section - Mass Fractions

	#201	#202	#203	#204	#204R	#205	#206	#207	#208	#209	#210	#211	#212
Temperature F	109	120	75	104	104	108	115.2	113.6	113.6	103	122.8	122.8	205
Pressure psi	16.9	135	20	16.8	16.8	14.5	71.2	14.5	16.5	16.5	16.5	35	35
Vapor Frac	0.999	0	0	0	0	0	0	0	0	0	0	0	0.007
Mole Flow lbmol/hr	2926.442	162.529	0.388	20212.43	20234.85	66411.55	154.038	66565.87	66565.87	66565.16	20388.4	20388.4	20472.12
Mass Flow lb/hr	86980	2928	17.333	417511.3	417761.5	1.20E+06	2777.42	1.20E+06	1.20E+06	1.20E+06	434149.1	434149.1	434149.1
Volume Flow cuft/hr	1.05E+06	47.426	0.271	6.79E+03	6798.54	19657.04	4.50E+01	19412.4	19412.29	19365.38	7202.798	7202.557	35776.93
Enthalpy MMBtu/hr	-94.069	-19.858	-0.046	-2507.879	-2510.509	-8123.753	-18.838	-8142.591	-8142.582	-8155.253	-2582.308	-2582.275	-2547.56
Mass Frac													
H2O	0.045	1	0.154	0.826	0.827	0.999	0.999	0.999	0.999	0.999	0.798	0.798	0.798
MEA			0.846	0.097	0.097	13 PPM	912 PPB	35 PPM	35 PPM	31 PPM	0.019	0.019	0.042
H2S											trace		
CO2	0.215			484 PPB	483 PPB	8 PPM	582 PPM	19 PPM	19 PPM	16 PPM	92 PPM	92 PPM	0.009
HCO3-	trace			904 PPM	903 PPM	377 PPM	321 PPM	370 PPM	370 PPM	375 PPM	0.011	0.011	0.011
MEACOO-				0.044	0.044	17 PPM	132 PPB	6 PPM	6 PPM	6 PPM	0.096	0.096	0.077
MEA+			992 PPB	0.027	0.027	399 PPM	327 PPM	383 PPM	383 PPM	388 PPM	0.07	0.07	0.058
CO3-2				107 PPM	107 PPM	2 PPM	22 PPB	909 PPB	908 PPB	1 PPM	312 PPM	312 PPM	71 PPM
HS-											trace		
S-2											trace		
H3O+	trace	8 PPB		trace	trace	trace	28 PPB	trace	trace	trace	trace	trace	trace
OH-	trace	8 PPB	272 PPB	2 PPM	2 PPM	171 PPB	2 PPB	79 PPB	79 PPB	70 PPB	372 PPB	372 PPB	625 PPB
O2	0.035			4 PPB	4 PPB		16 PPM	37 PPB	37 PPB	37 PPB	113 PPM	113 PPM	113 PPM
N2	0.704			11 PPB	11 PPB		47 PPM	109 PPB	109 PPB	109 PPB	881 PPM	881 PPM	881 PPM
AR	107 PPM			trace	trace		53 PPB	trace	trace	trace	365 PPB	365 PPB	365 PPB
CO	169 PPM			trace	trace		15 PPB	trace	trace	trace	243 PPB	243 PPB	243 PPB
HSS				0.004	0.004	62 PPM	46 PPM	62 PPM	62 PPM	62 PPM	0.004	0.004	0.004
H3N													
PARTIC													
NO2													
NAOH													
SO2	2 PPB			trace	trace		trace	trace	trace	trace	trace	trace	trace
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 4 Stream Table - CO2 Recovery Section - Mass Fractions

	#213	#214	#215	#216	#217	#218	#219	#220	#221	#222	#223	#224	#225
Temperature F	318.4	105.2	201.1	105	105.2	239.6	126.3	126.3	126.3	126.3	126.3	114.5	126.4
Pressure psi	58.7	46.2	25.7	26.2	46.2	28.7	28.7	58.7	58.7	58.7	58.7	25	25
Vapor Frac	1	0	1	0	0	0	0	0	0	0	0	0	0
Mole Flow lbmol/hr	34.691	144.425	562.768	230.358	85.924	20308.06	20306.67	20306.67	56.859	20.307	20229.51	5.356	20234.86
Mass Flow lb/hr	667.435	2608.339	18178.89	4160.293	1551.789	419247.8	419247.8	419247.8	1173.894	419.248	417654.6	106.929	417761.5
Volume Flow cuft/hr	4834.157	42.213	154072.9	67.33	25.114	7189.247	6866.097	6865.716	19.224	6.866	6.84E+03	1.728	6.84E+03
Enthalpy MMBtu/hr	-3.541	-17.697	-76.154	-28.227	-10.528	-2467.643	-2511.037	-2510.986	-7.031	-2.511	-2501.444	-0.654	-2502.098
Mass Frac													
H2O	0.908	0.996	0.242	0.996	0.996	0.826	0.827	0.827	0.827	0.827	0.827	0.862	0.827
MEA	0.078	2 PPM	213 PPM	2 PPM	2 PPM	0.1	0.097	0.097	0.097	0.097	0.097	0.135	0.097
H2S			trace			trace							
CO2	0.012	0.002	0.734	0.002	0.002	147 PPM	1 PPM	1 PPM	1 PPM	1 PPM	1 PPM	1 PPB	1 PPM
HCO3-		928 PPM		928 PPM	928 PPM	0.004	0.001	0.001	0.001	0.001	0.001	29 PPM	0.001
MEACOO-		815 PPB		813 PPB	815 PPB	0.039	0.043	0.043	0.043	0.043	0.043	0.002	0.043
MEA+		944 PPM		944 PPM	944 PPM	0.027	0.027	0.027	0.027	0.027	0.027	0.001	0.027
CO3-2		67 PPB		67 PPB	67 PPB	15 PPM	78 PPM	78 PPM	78 PPM	78 PPM	78 PPM	15 PPM	78 PPM
HS-						trace							
S-2						trace							
H3O+		32 PPB		32 PPB	32 PPB	trace	trace	trace	trace	trace	trace	trace	trace
OH-		2 PPB		2 PPB	2 PPB	1 PPM	2 PPM	2 PPM	2 PPM	2 PPM	2 PPM	35 PPM	2 PPM
O2	6 PPM	46 PPM	0.003	46 PPM	46 PPM	trace	trace	trace	trace	trace	trace	13 PPM	4 PPB
N2	19 PPM	136 PPM	0.021	136 PPM	136 PPM	trace	trace	trace	trace	trace	trace	39 PPM	11 PPB
AR	22 PPB	154 PPB	9 PPM	154 PPB	154 PPB	trace	trace	trace	trace	trace	trace	45 PPB	trace
CO	6 PPB	44 PPB	6 PPM	44 PPB	44 PPB	trace	trace	trace	trace	trace	trace	13 PPB	trace
HSS	0.002	134 PPM	31 PPM	134 PPM	134 PPM	0.004	0.004	0.004	0.004	0.004	0.004	39 PPM	0.004
H3N													
PARTIC													
NO2													
NAOH													
SO2	trace	1 PPB	2 PPB	1 PPB	1 PPB	trace	trace	trace	trace	trace	trace	trace	trace
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 4 Stream Table - CO2 Recovery Section - Mass Fractions

	#226	#227	#228	#229	#230	#231	#232	#233	#234	#235	#251	#252	#253
Temperature F	75.1	115.2	115.2	115.2	115.2	115.3	122	120.6	120.6	120.6	103	108	108
Pressure psi	25	71.2	71.2	71.2	71.2	81.2	58.7	68.7	68.7	68.7	16.5	14.5	14.5
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	1	1
Mole Flow lbmol/hr	0.388	248.452	14.907	4.969	74.536	74.536	35.21	427.225	341.78	85.445	66232.31	2530.317	71.628
Mass Flow lb/hr	17.333	4479.789	268.787	89.596	1343.937	1343.937	688.035	8434.215	6747.372	1686.843	1.19E+06	71050.42	2054.81
Volume Flow cuft/hr	2.71E-01	72.554	4.353	1.451	21.766	2.18E+01	11.212	137.525	110.02	27.505	19268.53	1.06E+06	3.01E+04
Enthalpy MMBtu/hr	-0.046	-30.385	-1.823	-0.608	-9.116	-9.115	-4.334	-52.673	-42.139	-10.535	-8114.466	-42.001	-0.204
Mass Frac													
H2O	0.154	0.999	0.999	0.999	0.999	0.999	0.894	0.881	0.881	0.881	0.999	0.054	
MEA	0.846	912 PPB	912 PPB	912 PPB	912 PPB	915 PPB	0.059	0.066	0.066	0.066	30 PPM	2 PPB	
H2S													
CO2		583 PPM	583 PPM	583 PPM	583 PPM	583 PPM	1 PPM	1 PPM	1 PPM	1 PPM	16 PPM	0.075	0.028
HCO3-		321 PPM	321 PPM	321 PPM	321 PPM	321 PPM	0.001	0.001	0.001	0.001	374 PPM		
MEACOO-		132 PPB	132 PPB	132 PPB	132 PPB	132 PPB	0.026	0.031	0.031	0.031	6 PPM		
MEA+	991 PPB	327 PPM	327 PPM	327 PPM	327 PPM	327 PPM	0.017	0.02	0.02	0.02	387 PPM		
CO3-2		22 PPB	22 PPB	22 PPB	22 PPB	22 PPB	114 PPM	117 PPM	117 PPM	117 PPM	1 PPM		
HS-													
S-2													
H3O+		28 PPB	28 PPB	28 PPB	28 PPB	28 PPB	trace	trace	trace	trace	trace		
OH-	272 PPB	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	3 PPM	3 PPM	3 PPM	3 PPM	70 PPB		
O2		16 PPM	16 PPM	16 PPM	16 PPM	16 PPM	6 PPM	13 PPM	13 PPM	13 PPM	37 PPB	0.039	0.107
N2		47 PPM	47 PPM	47 PPM	47 PPM	47 PPM	18 PPM	38 PPM	38 PPM	38 PPM	109 PPB	0.832	0.865
AR		53 PPB	53 PPB	53 PPB	53 PPB	53 PPB	21 PPB	43 PPB	43 PPB	43 PPB	trace	119 PPM	340 PPM
CO		15 PPB	15 PPB	15 PPB	15 PPB	15 PPB	6 PPB	12 PPB	12 PPB	12 PPB	trace	198 PPM	240 PPM
HSS		46 PPM	46 PPM	46 PPM	46 PPM	46 PPM	0.003				62 PPM	18 PPB	
H3N													
PARTIC													
NO2													
NAOH													
SO2		trace	trace	trace	trace	trace	trace				trace	trace	42 PPB
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 4 Stream Table - CO2 Recovery Section - Mass Fractions

	#254	#255	#256	#257	#258	#259	#260	#261	#291	#292	#293	#294
Temperature F	128.8	103	318.4	115	108	126.4	104	105.2	108	105	77	120.6
Pressure psi	14.5	16.5	58.7	46.2	14.5	68.7	16.5	46.2	14.5	26.2	58.7	68.7
Vapor Frac	1	0	0	0	0	0	0	0	1	1	0	0
Mole Flow lbmol/hr	2781.407	332.826	0.708	248.452	66482.98	56.859	20545.25	230.358	2601.945	332.347	86.153	45.932
Mass Flow lb/hr	76340.13	5999.66	20.601	4479.789	1.20E+06	1173.894	423511	4160.293	73105.23	14018.6	1707.444	830.987
Volume Flow cuft/hr	1.21E+06	96.827	0.378	72.556	19448.48	19.224	6891.491	67.329	1.09E+06	76278.14	27.557	13.464
Enthalpy MMBtu/hr	-60.416	-40.776	-0.082	-30.386	-8130.71	-7.031	-2548.655	-28.226	-42.205	-52.687	-10.689	-5.611
Mass Frac												
H2O	0.092	0.999	0.46	0.999	0.997	0.827	0.829	0.996	0.052	0.018	0.876	0.994
MEA	31 PPM	30 PPM	0.525	907 PPB	13 PPM	0.097	0.095	2 PPM	2 PPB	trace	0.071	
H2S	trace											
CO2	0.07	16 PPM	8 PPM	583 PPM	47 PPM	1 PPM	484 PPB	0.002	0.074	0.951	126 PPB	
HCO3-		374 PPM	170 PPM	321 PPM	397 PPM	0.001	903 PPM	928 PPM			588 PPM	
MEACOO-		6 PPM	0.002	131 PPB	3 PPM	0.043	0.043	815 PPB			0.032	
MEA+		387 PPM	0.001	327 PPM	407 PPM	0.027	0.027	944 PPM			0.02	
CO3-2		1 PPM	trace	22 PPB	405 PPB	78 PPM	109 PPM	67 PPB			202 PPM	
HS-												
S-2												
H3O+		trace		28 PPB	2 PPB	trace	trace	32 PPB			trace	8 PPB
OH-		70 PPB	271 PPB	2 PPB	28 PPB	2 PPM	2 PPM	2 PPB			3 PPM	8 PPB
O2	0.04	37 PPB	7 PPB	16 PPM	183 PPM	trace	4 PPB	46 PPM	0.041	0.004	12 PPM	
N2	0.797	109 PPB	10 PPB	47 PPM	0.001	trace	12 PPB	136 PPM	0.832	0.027	37 PPM	
AR	120 PPM	trace	trace	53 PPB	582 PPB	trace	trace	154 PPB	126 PPM	11 PPM	42 PPB	
CO	191 PPM	trace		15 PPB	410 PPB		trace	44 PPB	199 PPM	8 PPM	12 PPB	
HSS	5 PPM	62 PPM	0.011	46 PPM	62 PPM	0.004	0.004	134 PPM	18 PPB	13 PPB	136 PPM	0.006
H3N												
PARTIC												
NO2												
NAOH												
SO2	1 PPB	trace		trace	trace	trace	trace	1 PPB	1 PPB	2 PPB		trace
NA+												
HSO3-												
SO3-2												
NANO3												
NANO2												
H2SO3												
NAHSO3												

ASPEN does not have a built in unit operations block to model the water wash section so it was modeled with a 2-phase flash block with ideal separators on the vapor and liquid streams to reclaim the water and shift trace impurities into the vented overhead stream.

The absorber bottoms stream is pumped and then passed through the primary process cross flow heat exchanger where it is further heated before entering the top of the stripping column where the carbon dioxide is stripped. This is an endothermic process and the energy required comes from the steam provided to the reboiler. The water vapor in the stripped carbon dioxide is mostly condensed and used as a reflux. The reflux serves to minimize amine vapors in the overhead. Any excess reflux is pumped to the make-up water tank. The condensed water will contain amine and must undergo treatment prior to disposal.

The stripping column is modeled using RadFrac and contains 12 equilibrium stages.

The stripper column overhead contains the relatively pure CO_2 product that is fed to the final purification and liquefaction section. The stripper bottoms stream passes through the primary process cross flow heat exchanger and most of the stream is mixed with additional recycle and makeup solution and then fed back to the absorber column. A portion of the bottoms stream is passed through a filter to remove undissolved solids. Most of this filtered stream is recycled to the absorber and a small fraction is purged.

The primary process heat exchanger (H-201) is modeled in ASPEN as two Heater blocks (H-201 and H-201B) with their heat duties matched through a calculator block that imposes a 25% heat loss in the exchanger.

Auxiliary Systems

Operating problems arise from corrosion, foaming and solvent solution degradation. Ethanolamines are not corrosive as such. The pH of monoethanolamine solution in water is basic. With carbon dioxide loadings in the range of operation envisaged, the pH is still basic. At the temperatures encountered, the carbon dioxide and degradation products cause corrosion. Stress corrosion cracking conditions are prevalent too. Several mechanisms are attributed to the corrosion that occurs in ethanolamine systems. Alleviation has been attempted by several measures:

- Relieving of stress by heat treatment of all carbon steel vessels and piping has been specified.
- Areas of high concentration of carbon dioxide such as the top of stripper, overhead piping, condenser and so forth are of austenitic stainless steel.
- Areas of high temperature operation, such as the reboiler, have austenitic stainless steel tubes.
- Use of steam at very moderate temperatures in the reboiler and reclaimer.
- Restricting velocities of carbon dioxide containing solvents.
- Use of stainless steel clad tubes in the reclaimer, where high concentration of degradation products and relatively high temperatures are encountered.
- Continuous removal of suspended solids by filtration, and of amine degradation products by distillation of a side stream.

- Use of a corrosion inhibitor available under a trade name, which is a filming type, high molecular weight amine.

Foaming of the MEA solution may occur in both the absorber and stripper columns. Since hydrocarbons are not expected in discernible amounts in the scrubbed flue gases, foaming may not cause a problem. However, foaming in the stripper column must be guarded against for any carry over would amount to contamination of carbon dioxide fed to the purification steps. Foaming may occur when the following conditions appear:

- A high percentage of solid impurities such as fly ash, etc., in the circulating amine solution.
- A high concentration of soluble impurities in the circulating amine solution. These are primarily heat stable salts, and accumulated salts from makeup water.
- Accidental entry of lubricants, presence of grease, or other hydrocarbons in the amine solution.
- Antifoam agent, if required, is pumped to the top of stripper.
- Care should be taken to use condensate or demineralized water for makeup and for any requirement for pump seal flush, etc., so as to minimize presence of microconstituents that might promote foaming.
- The corrosion inhibitor added to the rich solvent at the absorber outlet and at the top of the stripper functions as an antifoam agent also.

There are several causes for solution losses. These include entrainment, vapor losses and solution degradation. Entrainment losses from the absorber are minimized by a Chevron type mist eliminator between the absorption section and the wash section, and a wire mesh mist eliminator at the top of the absorber. Vapor losses are controlled by keeping the temperature of vent gases as low as practicable. MEA is thermally stable at the temperature employed (245°F) in the regeneration step. The degradation is oxidative, by reactions with carbon dioxide, with sulfur compounds and other impurities. MEA reacts with oxygen to form carboxylic acids (such as oxalic acid, formic acid, glycolic acid, etc.) and ammonia. These, as well as impurities such as chlorides and carbonyl sulfide, form simple thermally stable salts with amine. The stable acid salts can be dissociated by reaction with strong bases, such as sodium hydroxide or sodium carbonate whereby the amine is liberated and may be recovered by distillation. MEA reacts with carbon dioxide to form oxazolidone-2, 1-(2-Hydroxyethyl) imidazolidone-2 and N-(2-Hydroxyethyl)-ethylenediarnine. The ethylenediamine derivative is hard to regenerate, being a very strong base. This may promote corrosion, especially when a high partial pressure of carbon dioxide is employed.

High boiling degradation products, heat stable salts, and sludge, are removed from the lean solution exiting the stripper by distillation of a small side stream (about 0.75 of the solvent flow). The stream is fed to a reclaimer that also serves as a reboiler, in a way, for it provides part of the stripping steam to the stripper. Sodium hydroxide is used to liberate the amine from the acid salts and minimize corrosion. This is added to the reclaimer after it is filled up with makeup (reflux) water, before heating begins. When steam is turned on, as the heating proceeds, steam and monoethanolamine boil off and enter the stripper. Distillation in the reclaimer is continuous until the accumulation of high boiling components raises the temperature to about 270 °F. This occurs perhaps in about four weeks of operating time. MEA remaining in the reclaimer is removed by adding water. The reclaimer residue is then pumped to the CO_2 plant waste water tank.

Precipitates, carry-over fly ash, and sludge are removed by filtration. A leaf type precoat pressure filter is used for about 20% of the solvent flow. Diatomaceous silica is used as a filter aid, in order to lengthen the filtration cycle while improving the quality of the filtered liquor. Because of the sizes and shapes of the diatom skeletons, the porosity is in the 0.9 range. When dispensed in the right proportion with the liquid being filtered, the resultant filter cake assumes the basic structure of the diatomaceous silica with adequate flow channels. "Precoat" is the thin layer of filter aid that is deposited on the filter medium prior to introducing the filter feed to the system. In this use, it protects the filter medium from fouling by the solids removed from the filter feed. It also provides a finer matrix to exclude particles from the filtrate, by bridging over the larger holes of the filter medium and filter-aid particles. "Body Feed" is the term used for filter aid added to the filter feed to increase the porosity of the filter cake. Body feed is added continuously during the filtration cycle. Upon completion of the filtration, the cake is cut off using teflon blades, and discharged in the dry form automatically.

<u>ASPEN Unit Operations Blocks</u>
Following is a description of each ASPEN Unit Operations Block in the simulation.

C-201 – Absorber Column
RadFrac Block, no condenser or reboiler, 10 equilibrium stages, Stage 1 pressure 14.5 psia, Column pressure drop 2 psia

C-202 – Stripper Column
RadFrac Block, no condenser, kettle reboiler, 12 equilibrium stages, Reboiler duty 25,000,000 Btu/hr, Stage 1 pressure 25.7 psia, Column pressure drop 3 psia

D-201 – Recycle solvent flash drum
Flash2 Block, Vapor fraction 0.98, Pressure drop 3 psia

D-202 – Stripper column partial condenser
Flash2 Block, Temperature 105 °F, Pressure 26.2 psia

D-203 – Waste solvent holdup tank
Heater Block, Temperature 77 °F, Pressure drop 5 psia

D-204 – Makeup water holdup tank
Mixer Block, 0 pressure drop

D-205 – Makeup solution holdup tank
Mixer Block, 0 pressure drop

F-101 – Particulates filter
Sep Block, Split fractions 0.1 for H_2O, 1.0 for particulates in stream #294

H-201 – Water wash return cooler
Heater Block, Temperature 103 °F, Pressure drop 2 psia

H-202 – Primary MEA solution process heat exchanger, cold side
Heater Block, Temperature 205 °F, Pressure drop 3 psia

H-202B - Primary MEA solution process heat exchanger, hot side
Heater Block, Heat duty per calculated duty of H-202, Pressure drop 3 psia

H-204 – CO_2 lean solvent recycle cooler
Heater Block, Temperature 104 °F, Pressure 16.8 psia

M-201 – Specialty ASPEN block for water wash recycle splitter
FSplit Block, Split fractions 0.995 for 251, 0.005 for 255

M-202 – Absorber column solvent feed stream mixer
Mixer block, 0 pressure drop

M-203 – Makeup water stream splitter
FSplit Block, Split fractions 0.62 for #206, 0.06 for #228, 0.02 for #229, 0.30 for #230

M-204 – Filtrate recycle splitter
FSplit Block, Split fractions 0.80 for #234, 0.20 for #235

M-205 – Stripper column solution recycle splitter
FSplit Block, Split fractions 0.627 for #214, 0.373 for #217

M-206 – CO_2 lean recycle solution splitter
FSplit Block, Split fractions 0.0028 for #221, 0.001 for #222, 0.9962 for #223

M-207 – CO_2 lean recycle solution mixer
Mixer block, 0 pressure drop

M-208 – Stripper column makeup solution mixer
Mixer block, 0 pressure drop

P-201 – CO_2 rich solvent pump
Pump Block, Discharge pressure 38 psia, Driver efficiency 0.97

P-202 – Water wash recycle pump
Pump Block, Pressure increase 2 psia, Driver efficiency 0.97

P-203 – CO_2 lean solvent filtrate pump
Pump Block, Pressure increase 10 psia, Driver efficiency 0.97

P-204 – Stripper column solution recycle pump
Pump Block, Pressure increase 20 psia, Driver efficiency 0.97

P-205 – CO_2 lean solvent pump
Pump Block, Discharge pressure 30 psia, Driver efficiency 0.97

P-206 – Water makeup from filter pump
Pump Block, Pressure increase 10 psia, Driver efficiency 0.97

P-207 – Makeup solution feed pump
Pump Block, Pressure increase 5 psia, Driver efficiency 0.97

P-208 – Makeup water feed/recycle pump
Pump Block, Pressure increase 25 psia, Driver efficiency 0.97

ZSEPCOR2 – Specialty ASPEN block for water wash model
Mixer Block, 0 pressure drop

ZSEPCORR – Specialty ASPEN block for water wash model
Sep Block, Split fractions 1.0 for H_2S, CO_2, O_2, N_2, Ar, CO in stream #253

ZWATWASH – Specialty ASPEN block for water wash model
Flash2 Block, Temperature 108 °F, 0 pressure drop

ZWMAKEUP – Specialty ASPEN block for water wash model
Mixer Block, 0 pressure drop

ASPEN Auxiliary Blocks
PRIMHTQ is a calculator block that sets the heat stream Q-H202B based on the calculated outlet heat stream from block H-202 with a 25% heat loss imposed.

Simulation Convergence
Convergence of the ASPEN simulation is achieved through five Convergence blocks, all using the bounded Wegstein method. The primary recycle loop for the MEA recycle solution also contains three nested recycle iterations for the solution makeup, water makeup, and the convergence loop to solve the water wash model within the absorber. This nesting requires a convergence tolerance on the water wash loop approximately one order of magnitude tighter than the outer loops. All Convergence block tolerances need to be 0.0001 or less. Otherwise, the bounded Wegstein method cannot converge the materials flows accurately enough to satisfy the charge balance constraints in the various unit operations blocks.

The calculation sequence is:

P-207
Convergence Block CSOLVRE1
Convergence Block CWWWATRE
M-201 M-202 C-201 P-201 PRIMHTQ H-202
Convergence Block CRECSOLV
D-201
Convergence Block CSOLVREF
C-202, D-202, P-204, M-206

D-205, P-208, ZWATWASH, ZSEPCORR, ZWMAKEUP, H-203, P205

M-207 M-203 M-210 P-202 H-201

ZSEPCOR2, D-204, P-209, M-209, P-206, H-204, P-210
Convergence Block CFSOLVRE
F-101, M-205

D-203

CO_2 Purification and Liquefaction Section

The process flow diagram for the CO_2 Purification and Liquefaction Section is shown in Figure 3. The calculated stream data is provided in Tables 5 and 6. The feed stream is assumed to be the overhead stream from the MEA stripping column from the CO_2 Recovery Section. The simulation will run with other inlet stream compositions but the physical property models are based on the assumption that the streams are predominantly CO_2.

For this section, an electrolyte-based physical property model is not justified. Rather, the base physical property model selected from ASPEN was the Redlich-Kwong-Suave cubic equation of state with Boston-Mathias alpha function (RKS-BM). This property method is recommended for gas-processing applications with nonpolar or mildly polar mixtures.

Carbon dioxide is liquefied at less than 300 psig and minus 12°F, therefore, it is necessary to dehydrate the carbon dioxide to a water dew point of minus 40°F or lower, to avoid freeze out of water on the heat transfer surfaces. Dehydration is accomplished using activated alumina as a desiccant. A short guard bed of activated carbon is provided to act as a filter and adsorb any lubricating oil vapor, which could contaminate the desiccant. Carbon dioxide from the recovery unit at 105°F is cooled to about 50°F. The condensed water serves to scrub out any carried over amine or decomposition products such as ammonia.

To maintain computational stability in the purification column, the feed stream is passed through a Separator block to remove excess quantities of noncondensible gases, particularly O_2 and N_2.

CO_2 is then compressed to about 315 psia in a compound compressor. The CO_2 compressor is modeled as a 4-stage compressor with intercoolers that cool the intermediate compressed gas stream to 200 °F between each stage. The third stage pressure is set to 218 psia to allow a small recycle gas stream to enter at stage 4. The stage 4 outlet pressure is set to 315 psia. The compressor was modeled using the isentropic efficiency method with an isentropic efficiency of 0.80 used for each stage. A mechanical efficiency of 0.97 was assumed.

The compressed gas is fed to a zinc oxide absorber to remove any residual sulfur compound. This step is prior to removal of the heat of compression, because the chemical reaction in this guard bed occurs at an elevated temperature. The sulfur removal unit is modeled in ASPEN as a Separator block with 100% efficiency in the removal of all sulfur compounds.

After cooling in successive exchangers, carbon dioxide passes through a water knockout drum and oil coalescer, before entering the dehydrators. The dryer is modeled as a Separator block with an assumed 100% efficiency in removal of water vapor. From here, the gas flows through dust filters and a mercury guard bed, before entering the carbon dioxide stripper reboiler. The gas is cooled in the reboiler and then condensed in the main CO_2 condenser.

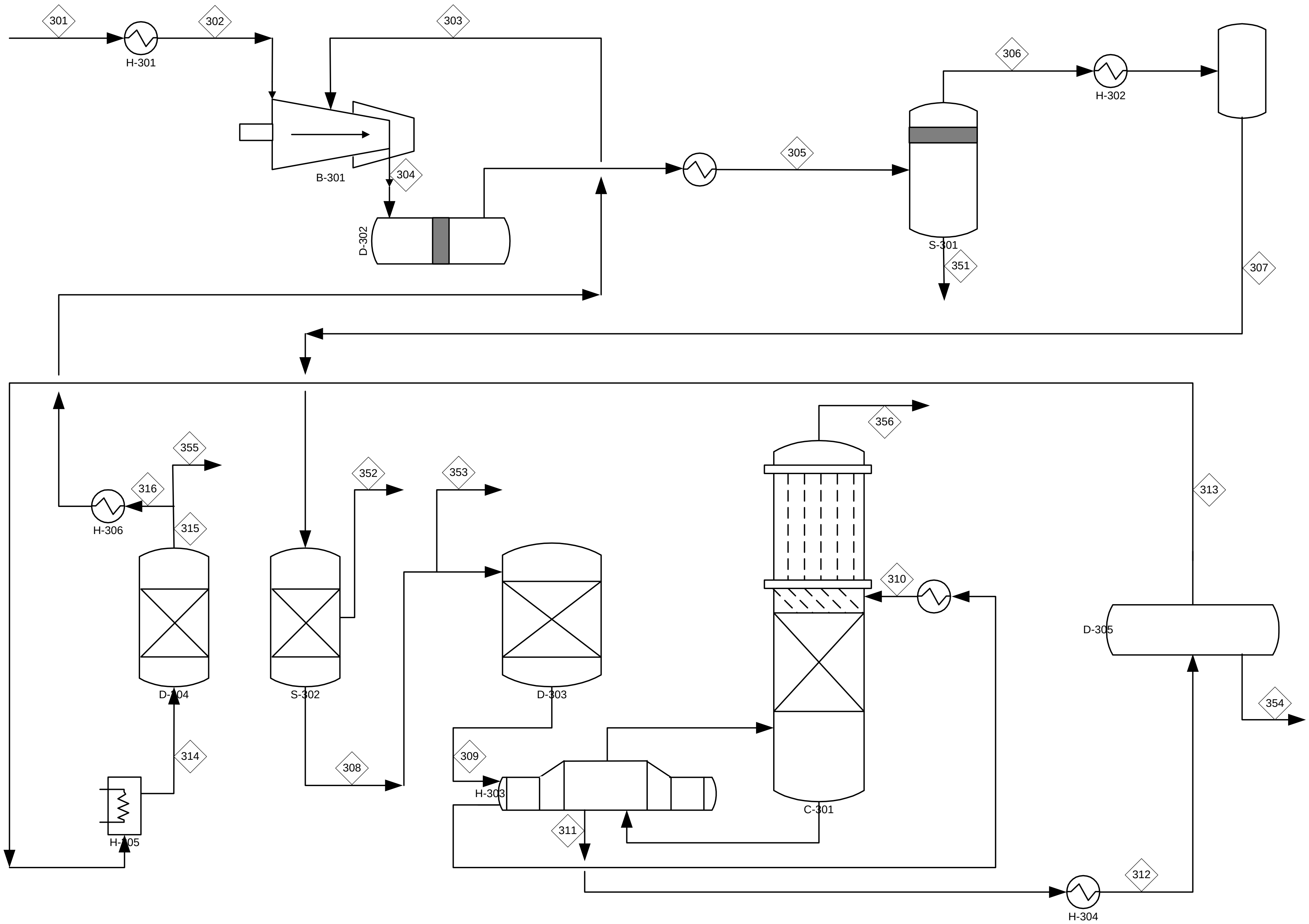

Figure 3 CO_2 Purification and Liquefaction Section

Table 5 Stream Table - CO2 Purification and Liquefaction Section - Mass Flows

	#301	#302	#303	#304	#305	#306	#307	#308	#309	#310	#311	#312	#313
Temperature F	105	91.8	480	661.5	171	171	50	50	55.7	-10	-0.7	-15	-14.6
Pressure psi	26.2	17.5	218	315	315	315	321	321	321	310	308	298	244.4
Vapor Frac	1	1	1	1	0.98	0.98	0.957	1	1	0	0	0	1
Mole Flow lbmol/hr	412.475	398.514	4.296	402.809	402.809	402.809	402.809	366.391	366.391	366.391	357.964	357.964	4.296
Mass Flow lb/hr	17460.6	17069.93	187.456	17257.39	17257.39	17257.39	17257.39	16101.26	16101.26	16101.26	15748.05	15748.05	187.456
Volume Flow cuft/hr	9.47E+04	133999.4	197.876	1.52E+04	7887.557	7887.557	5.67E+03	5379.605	5449.595	273.923	242.721	263.049	70.022
Enthalpy MMBtu/hr	-66.064	-66.05	-0.693	-64.439	-66.71	-66.71	-67.381	-62.006	-62.006	-64.255	-62.881	-63.011	-0.715
Mass Flow lb/hr													
H2O	319.229	308.695	trace	308.695	308.694	308.694	308.689	0.006	0.006	0.006	0.006	0.006	trace
MEA	trace												
H2S													
CO2	16719.04	16719.03	184.477	16903.5	16903.5	16903.5	16903.5	16058.33	16058.33	16058.33	15736.6	15736.6	184.477
HCO3-			trace	< 0.001	0.003	0.003	0.011			trace	trace	trace	trace
MEACOO-													
MEA+													
CO3-2					trace	trace	trace						
HS-													
S-2													
H3O+			trace	trace	0.001	0.001	0.003			trace	trace	trace	trace
OH-				trace	trace	trace	trace						
O2	47.736	4.774	0.565	5.338	5.338	5.338	5.338	5.071	5.071	5.071	3.451	3.451	0.565
N2	374.332	37.433	2.414	39.848	39.848	39.848	39.848	37.855	37.855	37.855	7.997	7.997	2.414
AR	0.155	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
CO	0.103	< 0.001	trace	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	trace
HSS	< 0.001	< 0.001		< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	
H3N													
PARTIC													
NO2													
NAOH													
SO2	< 0.001	trace		trace	trace								
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 5 Stream Table - CO2 Purification and Liquefaction Section - Mass Flows

	#314	#315	#316	#331	#332	#333	#334	#335	#351	#352	#353	#354	#355
Temperature F	500	500	500	91.8	91.8	200	522.4	50	171	50	50	-14.6	
Pressure psi	228	228	228	17.5	17.5	215	215	321	315	321	321	244.4	
Vapor Frac	1	1	1	1	0.999	1	0.979	1	0	0	1	0	
Mole Flow lbmol/hr	4.296	4.296	4.296	412.475	399.099	398.514	402.809	385.675	< 0.001	17.135	19.284	353.668	0
Mass Flow lb/hr	187.456	187.456	187.456	17460.6	17080.48	17069.93	17257.39	16948.7	< 0.001	308.689	847.435	15560.59	0
Volume Flow cuft/hr	193.372	193.372	193.372	138725.2	133999.6	12615.63	19125.69	5662.742	< 0.001	4.941	2.83E+02	260.77	0.00E+00
Enthalpy MMBtu/hr	-0.692	-0.692	-0.692	-66.109	-66.121	-65.723	-64.889	-65.269	> -0.001	-2.115	-3.263	-62.268	
Mass Flow lb/hr													
H2O	trace	trace	trace	319.229	319.229	308.695	308.695	0.006		308.689	< 0.001	0.006	
MEA				trace	trace								
H2S													
CO2	184.477	184.477	184.477	16719.04	16719.04	16719.03	16903.5	16903.5			845.175	15552.12	
HCO3-	trace	trace	trace		< 0.001		< 0.001					trace	
MEACOO-													
MEA+					trace								
CO3-2					trace								
HS-													
S-2													
H3O+	trace	trace	trace		< 0.001		trace			trace		trace	
OH-					trace		trace			trace			
O2	0.565	0.565	0.565	47.736	4.774	4.774	5.338	5.338			0.267	2.886	
N2	2.414	2.414	2.414	374.332	37.433	37.433	39.848	39.848			1.992	5.583	
AR	< 0.001	< 0.001	< 0.001	0.155	< 0.001	< 0.001	< 0.001	< 0.001			trace	< 0.001	
CO	trace	trace	trace	0.103	< 0.001	< 0.001	< 0.001	< 0.001			trace	< 0.001	
HSS				< 0.001	< 0.001	< 0.001	< 0.001	< 0.001			trace	< 0.001	
H3N													
PARTIC													
NO2													
NAOH													
SO2				< 0.001	trace	trace	trace		trace				
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 5 Stream Table - CO_2 Purification and Liquefaction Section - Mass Flows

	#356	#357	#358
Temperature F	-9.3	91.8	91.8
Pressure psi	308	17.5	17.5
Vapor Frac	1	0	1
Mole Flow lbmol/hr	8.427	0.585	13.376
Mass Flow lb/hr	353.213	10.549	380.118
Volume Flow cuft/hr	1.08E+02	0.17	4521.965
Enthalpy MMBtu/hr	-1.248	-0.072	0.001
Mass Flow lb/hr			
H2O	trace	10.534	
MEA			
H2S			
CO2	321.734	0.015	
HCO3-	trace	< 0.001	
MEACOO-			
MEA+		trace	
CO3-2			
HS-			
S-2			
H3O+	trace	< 0.001	
OH-			
O2	1.62	< 0.001	42.962
N2	29.858	< 0.001	336.899
AR	< 0.001	trace	0.154
CO	< 0.001	trace	0.102
HSS	trace	< 0.001	
H3N			
PARTIC			
NO2			
NAOH			
SO2		trace	< 0.001
NA+			
HSO3-			
SO3-2			
NANO3			
NANO2			
H2SO3			
NAHSO3			

Table 6 Stream Table - CO2 Purification and Liquefaction Section - Mass Fractions

	#301	#302	#303	#304	#305	#306	#307	#308	#309	#310	#311	#312	#313
Temperature F	105	91.8	480	661.5	171	171	50	50	55.7	-10	-0.7	-15	-14.6
Pressure psi	26.2	17.5	218	315	315	315	321	321	321	310	308	298	244.4
Vapor Frac	1	1	1	1	0.98	0.98	0.957	1	1	0	0	0	1
Mole Flow lbmol/hr	412.475	398.514	4.296	402.809	402.809	402.809	402.809	366.391	366.391	366.391	357.964	357.964	4.296
Mass Flow lb/hr	17460.6	17069.93	187.456	17257.39	17257.39	17257.39	17257.39	16101.26	16101.26	16101.26	15748.05	15748.05	187.456
Volume Flow cuft/hr	9.47E+04	133999.4	197.876	1.52E+04	7887.557	7887.557	5.67E+03	5379.605	5449.595	273.923	242.721	263.049	70.022
Enthalpy MMBtu/hr	-66.064	-66.05	-0.693	-64.439	-66.71	-66.71	-67.381	-62.006	-62.006	-64.255	-62.881	-63.011	-0.715
Mass Frac													
H2O	0.018	0.018	4 PPB	0.018	0.018	0.018	0.018	374 PPB	374 PPB	374 PPB	382 PPB	382 PPB	4 PPB
MEA	trace												
H2S													
CO2	0.958	0.979	0.984	0.979	0.979	0.979	0.979	0.997	0.997	0.997	0.999	0.999	0.984
HCO3-			trace	1 PPB	164 PPB	164 PPB	622 PPB			trace	trace	trace	trace
MEACOO-													
MEA+													
CO3-2					trace	trace	trace						
HS-													
S-2													
H3O+			trace	trace	51 PPB	51 PPB	194 PPB			trace	trace	trace	trace
OH-				trace	trace	trace	trace						
O2	0.003	280 PPM	0.003	309 PPM	309 PPM	309 PPM	309 PPM	315 PPM	315 PPM	315 PPM	219 PPM	219 PPM	0.003
N2	0.021	0.002	0.013	0.002	0.002	0.002	0.002	0.002	0.002	0.002	508 PPM	508 PPM	0.013
AR	9 PPM	9 PPB	99 PPB	10 PPB	10 PPB	10 PPB	10 PPB	10 PPB	10 PPB	10 PPB	7 PPB	7 PPB	99 PPB
CO	6 PPM	6 PPB	49 PPB	6 PPB	6 PPB	6 PPB	6 PPB	7 PPB	7 PPB	7 PPB	2 PPB	2 PPB	49 PPB
HSS	18 PPB	2 PPB		2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	2 PPB	
H3N													
PARTIC													
NO2													
NAOH													
SO2	2 PPB	trace		trace	trace								
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 6 Stream Table - CO2 Purification and Liquefaction Section - Mass Fractions

	#314	#315	#316	#331	#332	#333	#334	#335	#351	#352	#353	#354	#355
Temperature F	500	500	500	91.8	91.8	200	522.4	50	171	50	50	-14.6	
Pressure psi	228	228	228	17.5	17.5	215	215	321	315	321	321	244.4	
Vapor Frac	1	1	1	1	0.999	1	0.979	1	0	0	1	0	
Mole Flow lbmol/hr	4.296	4.296	4.296	412.475	399.099	398.514	402.809	385.675	< 0.001	17.135	19.284	353.668	0
Mass Flow lb/hr	187.456	187.456	187.456	17460.6	17080.48	17069.93	17257.39	16948.7	< 0.001	308.689	847.435	15560.59	0
Volume Flow cuft/hr	193.372	193.372	193.372	138725.2	133999.6	12615.63	19125.69	5662.742	< 0.001	4.941	2.83E+02	260.77	0.00E+00
Enthalpy MMBtu/hr	-0.692	-0.692	-0.692	-66.109	-66.121	-65.723	-64.889	-65.269	> -0.001	-2.115	-3.263	-62.268	
Mass Frac													
H2O	4 PPB	4 PPB	4 PPB	0.018	0.019	0.018	0.018	374 PPB		1	374 PPB	387 PPB	
MEA				trace	trace								
H2S													
CO2	0.984	0.984	0.984	0.958	0.979	0.979	0.979	0.997			0.997	0.999	
HCO3-	trace	trace	trace		5 PPB		1 PPB					trace	
MEACOO-													
MEA+					trace								
CO3-2					trace								
HS-													
S-2													
H3O+	trace	trace	trace		2 PPB		trace			3 PPB		trace	
OH-					trace		trace			3 PPB			
O2	0.003	0.003	0.003	0.003	279 PPM	280 PPM	309 PPM	315 PPM			315 PPM	185 PPM	
N2	0.013	0.013	0.013	0.021	0.002	0.002	0.002	0.002			0.002	359 PPM	
AR	99 PPB	99 PPB	99 PPB	9 PPM	9 PPB	9 PPB	10 PPB	10 PPB			10 PPB	6 PPB	
CO	49 PPB	49 PPB	49 PPB	6 PPM	6 PPB	6 PPB	6 PPB	7 PPB			7 PPB	2 PPB	
HSS				18 PPB	18 PPB	2 PPB	2 PPB	2 PPB			2 PPB	2 PPB	
H3N													
PARTIC													
NO2													
NAOH													
SO2				2 PPB	trace	trace	trace		1				
NA+													
HSO3-													
SO3-2													
NANO3													
NANO2													
H2SO3													
NAHSO3													

Table 6 Stream Table - CO_2 Purification and Liquefaction Section - Mass Fractions

	#356	#357	#358
Temperature F	-9.3	91.8	91.8
Pressure psi	308	17.5	17.5
Vapor Frac	1	0	1
Mole Flow lbmol/hr	8.427	0.585	13.376
Mass Flow lb/hr	353.213	10.549	380.118
Volume Flow cuft/hr	1.08E+02	0.17	4521.965
Enthalpy MMBtu/hr	-1.248	-0.072	0.001
Mass Frac			
H2O	4 PPB	0.999	
MEA			
H2S			
CO2	0.911	0.001	
HCO3-	trace	8 PPM	
MEACOO-			
MEA+		176 PPB	
CO3-2			
HS-			
S-2			
H3O+	trace	2 PPM	
OH-			
O2	0.005	3 PPM	0.113
N2	0.085	9 PPM	0.886
AR	154 PPB	trace	406 PPM
CO	207 PPB	trace	270 PPM
HSS	trace	26 PPM	
H3N			
PARTIC			
NO2			
NAOH			
SO2		trace	72 PPB
NA+			
HSO3-			
SO3-2			
NANO3			
NANO2			
H2SO3			
NAHSO3			

Summarizing, the purification of CO_2 is accomplished by the following steps:

- Compression, followed by cooling that removes water. The condensed water also scrubs out any carried over impurities such as amine, ammonia, etc.
- Removal of any residual sulfur compounds in zinc oxide. The zinc oxide is Katalco Type.
- Activated alumina removes moisture as well as oxides of nitrogen.
- A guard adsorber, containing sulfur impregnated activated carbon, captures any mercury that may not be retained in the solvent solution of the recovery unit. Mercury escapes in its elemental form in the flue gases.

About 95% of the carbon dioxide passing through the main condenser is liquefied, by lowering the temperature to -10°F. The liquefied carbon dioxide and uncondensed vapors then enter the top of the distillation column. Overhead vapors from this column are further condensed in a shell and tube condenser. Liquid is refluxed, and uncondensed vapors are vented out. Product carbon dioxide from the stripping column bottom is subcooled to about -15°F prior to storage.

The distillation column is modeled using RadFrac and contains 10 equilibrium stages. The condenser pressure is set to 308 psia and the column operates with a distillate to feed ratio or 0.023. The column overhead stream is vented. The bottoms stream is 99.9% pure CO_2. It is flashed to 244 psia and the liquid taken as the CO_2 product stream. The vapor product from the flash is recycled to the compressor.

<u>ASPEN Unit Operations Blocks</u>

Following is a description of each ASPEN Unit Operations Block in the simulation.

B-301A – CO_2 compressor, initial stages
MCompr Block, Discharge pressure 218 psia, Isentropic efficiency 0.84, interstage gas cooling temperature 200 °F, Mechanical efficiency 0.97

B-301B – CO_2 compressor, final stage
Compr Block, Discharge pressure 330 psia, Isentropic efficiency 0.84, Mechanical efficiency 0.97

C-301 – Distillation Column
RadFrac Block, 10 equilibrium stages, no condenser, kettle reboiler, Distillate to feed ratio 0.023, Stage 1 pressure 308 psia

D-301 – Gas feed stream vapor/liquid separator
Flash2 Block, Adiabatic operation, 0 pressure drop

D-302 – Compressed gas cooler, stage 1
Heater Block, Temperature 171 F, -3 psia pressure drop

D-303 – Dehydrated CO_2 holdup tank
Mixer Block, Adiabatic operation, 0 pressure drop

D-304 – Recycle gas dryer, mixer portion
Mixer Block, Adiabatic operation, 0 pressure drop

D-305 – CO_2 product flash
Flash2 Block, Outlet pressure 244.4 psia, Vapor fraction 0.012

H-301 – Feed gas stream cooler
Heater Block, Pressure 17.5 psia, Vapor fraction 1.0

H-302 – Compressed gas cooler, stage 2
Heater Block, Temperature 50 °F, Pressure 321 psia

H-303 – Dehydrated CO_2 cooler
Heater Block, Temperature –10 °F, Pressure 310 psia

H-304 – Primary CO_2 product cooler
Heater Block, Temperature -15 °F, -10 psia pressure drop

H-305 – Recycle CO_2 gas heater
Heater Block, Temperature 500 °F, Outlet pressure 228 psia

H-306 – Recycle CO_2 gas cooler
Temperature –20 °F, Pressure drop –10 psia

M-301 – Final stage CO_2 compressor feed stream mixer
Mixer Block, Adiabatic operation, 0 pressure drop

M-302 – Dehydrated CO_2 blowdown splitter
FSplit Block, Split fractions 0.95 for #308, 0.05 for #353

M-303 – Recycle CO_2 gas vent splitter
FSplit Block, Split fractions 1.0 for 316, 0.0 for #355

M-304 – ASPEN specialty block for mixer CO_2 compressor work streams
Mixer Block

S-301 – Desulfurizer
Sep Block, Split fractions 1.0 for H_2S, HS-, S^{-2}, SO_2, HSO3-, SO_3^{-2}, H_2SO_3 , $NaHSO_3$ in stream #351

S-302 – Compressed CO2 dehydrator
Sep Block, Split fractions 1.0 for H_{2O} in stream #352

ASPEN Auxiliary Blocks
There are no design specifications or calculator blocks used to control the simulation.

Simulation Convergence
Convergence of the recycle stream is achieved from a single Convergence block using the bounded Wegstein method and stream #313 as the tear stream.

The calculation sequence is:

H-301, S-303, D-301, B-301A, H-305, D-304
→ Convergence Block CPURREC1
M-303, H-306, M-301, B-301B, D-302, S-301, H-302, S-302, M-302, D-303, H-303, C-301, H-304, D-305

M-304

Results

Stream Tables are provided with the process flow diagrams for each section. In addition to the material flows, the following power streams and heat duties were calculated.

Table 7 Stream Table – Power Streams

Stream	Power (hp)
W-B101	734.2
W-P101	1.68
W-P102	0.14
W-P103	0.005
W-P104	0.097
W-P105	2.51
W-P106	0.81
W-P107	0.27
W-P201	15.2
W-P202	3.64
W-P203	0.049
W-P204	0.34
W-P205	20.36
W-P206	0.055
W-P207	0.001
W-P208	0.46
W-B301	791.2

Table 8 Stream Table – Heat Streams

Stream	Heat Duty (Btu/hr)
Q-H101	874,741
Q-H102	4,145,570
Q-H201	12,745,349
Q-H202	34,715,027
Q-H204	8,410,696
Q-H301	45,066
Q-H302	671,577
Q-H303	2,248,672
Q-H304	129,331
Q-H305	22,903
Q-H306	930

Appendix A - ASPEN Simulation Model Defaults

Item	Comments
Components	H_2O, MEA, H_2S, CO_2, HCO_3^-, $MEACOO^-$, MEA^+, CO_3^{-2}, HS^-, S^{-2}, H_3O^+, OH^-, O_2, N_2, Ar, CO, HSS, H_3N, PARTIC, NO_2, NaOH, SO_2, Na^+, HSO_3^-, SO_3^{-2}, $NaNO_3$, $NaNO_2$, $H2SO_3$, $NaHSO_3$
Physical Property	ELECNRTL (per MEA - Water - H2S - CO2 insert) for flue gas scrubbing and CO_2 recovery sections, RKS-BM for CO_2 purification and liquefaction section
Stream Class	Conventional
Units Set	Eng
Block Report	Total mass and energy balance Summary of user input & system defaults Block results
Stream Report	Mass flow, Mass fraction, CHEM_E TTF
Recycle Convergence	Bounded Wegstein Method Tolerance 0.0001
Calculation Sequence	Manual, User specified