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LLNL-TR-646154

Description of the Process Model for the Technoeconomic Evaluation of MEA versus Mixed Amines for Carbon Dioxide Removal from Stack Gas

D. A. Jones

November 13, 2013

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November 8, 2013

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Executive Summary

This model description is supplemental to the Lawrence Livermore National Laboratory (LLNL) report LLNL-TR-642494, *Technoeconomic Evaluation of MEA versus Mixed Amines for CO_2 Removal at Near-Commercial Scale at Duke Energy Gibson 3 Plant*. We describe the assumptions and methodology used in the Laboratory's simulation of its understanding of Huaneng's novel amine solvent for CO_2 capture with 35% mixed amine. The results of that simulation have been described in LLNL-TR-642494.

The simulation was performed using ASPEN 7.0. The composition of the Huaneng's novel amine solvent was estimated based on information gleaned from Huaneng patents. The chemistry of the process was described using nine equations, representing reactions within the absorber and stripper columns using the ELECTNRTL property method. As a rate-based ASPEN simulation model was not available to Lawrence Livermore at the time of writing, the height of a theoretical plate was estimated using open literature for similar processes. Composition of the flue gas was estimated based on information supplied by Duke Energy for Unit 3 of the Gibson plant. The simulation was scaled at one million short tons of CO_2 absorbed per year.

To aid stability of the model, convergence of the main solvent recycle loop was implemented manually, as described in the Blocks section below. Automatic convergence of this loop led to instability during the model iterations. Manual convergence of the loop enabled accurate representation and maintenance of model stability.

Background and Scope

This model description is supplemental to the report LLNL-TR-642494, *Technoeconomic Evaluation of MEA versus Mixed Amines for CO_2 Removal at Near-Commercial Scale at Duke Energy Gibson 3 Plant.* It is intended for a technical audience, to give more details on the decisions and rationale underlying the process simulations described in that report and used as the basis of the economic calculations also contained in said report.

Using Aspen Plus®, we have modeled a carbon capture plant capable of removing one million tons of carbon dioxide from a fraction of the flue gas generated by a US-based coal-fired power plant. Although much modeling effort has been made on the process of carbon capture using aqueous amine solvent,[1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15] [16] no plant has been built to this scale. We created a model of this plant to determine the size and cost of the equipment as well as operating costs. This report describes the Aspen model used to define the process. For a more complete description of the project, consult the original Technoeconomic Evaluation.[17]

We modeled the process using Aspen Plus, Version 7.0 without Rate-Based Distillation. Therefore, our model will calculate the results of the absorption and stripping columns assuming all species and phases are in equilibrium at each stage. According to studies by Freguia[18] and others, the equilibrium assumption is accurate for the stripping column, but not the absorption column. The result is the underprediction of the number of stages in the absorption column. As a temporary workaround for this situation, we used "Height Equivalent to a Theoretical Plate" (HETP)data from Freguia.

Setting Up the Simulation, Preliminary Calculations

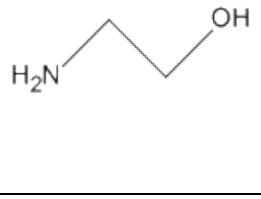
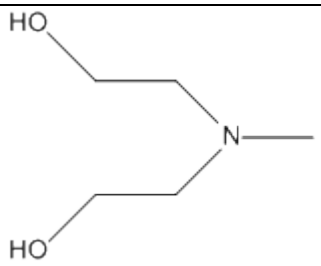
Since preliminary calculations must be made before entering the information into Aspen, it is useful to use Microsoft Excel for this purpose. It is also very helpful to export Aspen's results to Excel so that further calculations can be made and all the information is presented on one page. The design specifications of the plant are as follows:

- Remove and compress one million English tons of carbon dioxide per year from Unit 3 of Duke Energy's Gibson Station
- The carbon capture plant is to operate continuously 80% of the time
- The input flue gas is at one atmosphere pressure at 130°F (54.4°C) with the following molar composition:
  - 9.5% carbon dioxide
  - 15.5%% water
  - 67.6% nitrogen
  - 6.6% oxygen
  - 1.1 ppm hydrogen chloride
  - 63 ppm sulfur dioxide

To meet the removal specification, we must take 15,300 cubic feet per hour (cfh) or 937 cubic meters per hour of Duke's flue gas or 25.5% or the flue gas generated by Gibson Station Unit 3. These values were calculated using information provided by Duke Energy, and used as inputs to the Aspen simulation.

The purpose of the project is to evaluate Huaneng's proprietary amine mixture, comparing it with the baseline of a single amine, monoethanolamine (MEA), in water at a concentration of 30% by weight. Since we did not know the actual composition of the proprietary amine mixture, we chose the mixture in Huaneng's patent[19] that represented the largest deviation from MEA alone. The amines used in our model, MEA, methyldiethanolamine (MDEA), and 2-amino-2-methyl propan-1-ol (AMP), are included in Aspen's databanks. The amine mix we modeled was 50% MEA, 40% MDEA, and 10% AMP by weight. We compared two amine concentrations, 30% and 35% by weight in water. Table 1 shows the structural formulas for the three amines; following is the procedure we used to set up the simulation.

Table 1. Amines used in carbon capture process models

		
Monoethanolamine (MEA)	Methyl diethanolamine (MDEA)	2-amino-2-methyl propan-1-ol (AMP)

In setting up the simulation, Aspen leads us through the following steps, each of which is described in the remaining sections of this report:

- Draw the process flow diagram (PFD) by selecting the blocks, followed by the streams that connect these blocks
- Input the data:
  - In the SETUP section, describe the process and specify how the results are to be presented
  - In the COMPONENTS section, specify the chemicals that are involved in the process
  - In the PROPERTIES section, select the appropriate property data for the chemicals.
  - In the REACTIONS section, specify and balance the chemical reactions
  - In the BLOCKS section, set the parameters for all the unit operations
  - In the STREAMS section, set the properties for the appropriate streams
- Run the simulation

Process Flow Diagram (PFD)

The first step to setting up an Aspen simulation is to draw the PFD. Figure 1 is the PFD as drawn by Aspen based on blocks and streams we entered. This PFD is similar to that of the Huaneng process,[20] as

well as other amine-based carbon capture processes. A *block* is a piece of equipment or unit operation, such as a reactor or pump. A *stream* is the material in the piping to and from a block. We describe each block followed by the appropriate streams. Each block or stream is identified below by a descriptive title followed by its label on the PFD.

The diagram in Figure 1 describes the process as it would be operated, in a continuous loop with flue gas entering and cleaned gas and compressed CO_2 leaving. As mentioned below, for modeling stability, we separated the recycle stream, REC, into two streams REC and REC2 and manually adjusted the feed stream, AMINEFD, until the output stream, REC, and the input stream, REC2, were identical in composition and properties.

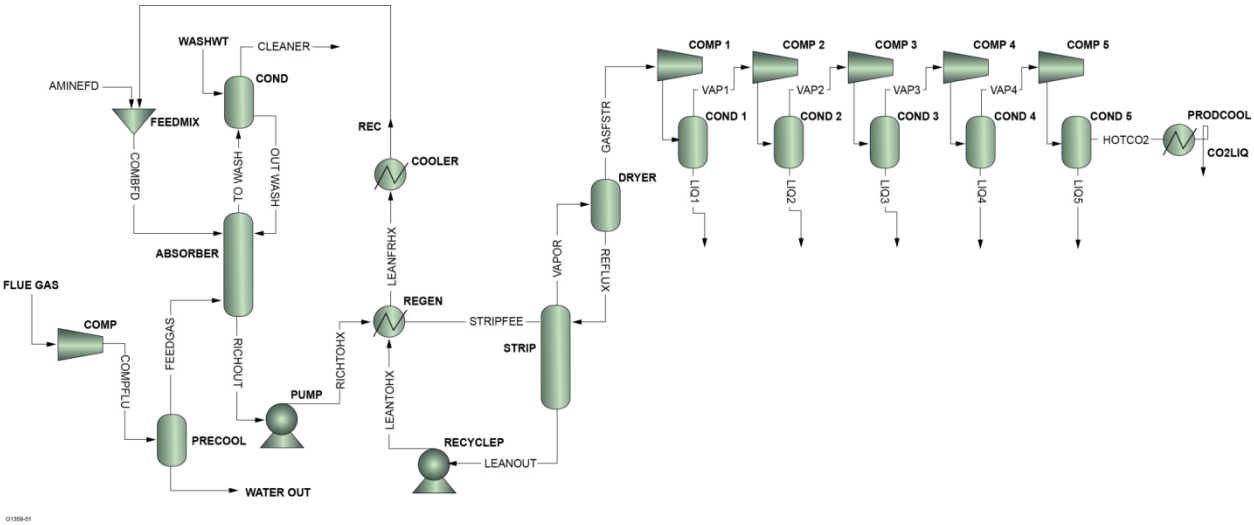


Figure 1. Carbon Capture Process as drawn by Aspen Plus

Data to Be Entered

Once the PFD is drawn, Aspen Plus opens the input sections in the following order:

Setup

The SETUP section asks for a project name and report options, among other information. We chose the results to be in metric units, both mass and molar. Duke Energy operates in English units and Huaneng operates in metric (SI) units, so either way, we would have to make conversions, which are not a problem after exporting the stream tables to Excel.

Components

The COMPONENTS section asks for a list of chemicals involved in the simulation. Because Aspen has been used for years to design amine-based carbon dioxide capture, all the chemicals in our simulations are contained in its databanks. Although the properties are specified in a later section, the Electrolyte Wizard is in this section. The Electrolyte Wizard uses the Electrolyte Non-Random-Two-Liquid

(ELECNRTL) property set, which handles the highly non-ideal case of electrolyte solutions at high concentration. The chemicals used in our simulations are given below. The chemicals entered into Aspen are shown in bold. The remaining species, all ionic, were added by the Electrolyte Wizard.

- **Carbon dioxide**
- **Water**
- **Nitrogen**
- **Oxygen**
- **Sulfur dioxide**
- **Hydrogen chloride**
- **Monoethanolamine (MEA)**
- **Methyl diethanolamine (MDEA)**
- **2-amino-2-methyl propan-1-ol (AMP)**
- Hydronium ion, H_3O^+
- Bicarbonate ion, HCO_3^-
- Chloride ion, Cl^-
- Carbonate ion, $CO_3=$
- Amine hydronium ions, $MEAH^+$, $MDEAH^+$, and $AMPH^+$
- Amine carbamate, $MEACOO^-$ only[a]
- Bisulfite ion, HSO_3^-
- Sulfite ion, $SO_3^=$

Properties

The PROPERTIES section asks for the property set to be used for the simulation. In our case, the property set, ELECNRTL, was specified in the components section.

[a] MEA is the only one of the three amines that forms a carbamate. Since only primary and secondary amines can form carbamates, MDEA, a tertiary amine, cannot. AMP, a primary amine, cannot form a stable carbamate because of steric hindrance, adjacent methyl groups interfering with carbamate formation.

Reactions

The REACTIONS section asks for the chemical reactions that take place in the process, either as REACTIONS, which are rate-controlled, or CHEMISTRY, which are equilibrium controlled. Because we did not have rate-based distillation, we used CHEMISTRY. The reactions are as follows.

1. $HCl + H_2O \leftrightarrow H_3O^+ + Cl^-$
2. $H_2O + MEAH^+ \leftrightarrow H_3O^+ + MEA$
3. $H_2O + HCO_3^- \leftrightarrow H_3O^+ + CO_3^=$
4. $H_2O + MEACOO^- \leftrightarrow MEA + HCO_3^-$
5. $H_2O + HSO_3^- \leftrightarrow H_3O + SO_3^=$
6. $2\ H_2O + SO_2 \leftrightarrow H_3O^+ + HSO_3^-$
7. $H_2O + MDEAH^+ \leftrightarrow H_3O^+ + MDEA$
8. $H_2O + AMPH^+ \leftrightarrow H_3O^+ + AMP$
9. $2\ H_2O + CO_2 \leftrightarrow H_3O^+ + HCO_3^-$

The equilibrium constants in Aspen's databanks were different from literature values. The expression for the equilibrium constant is:

$Ln\ K = A + B/T + C\ lnT + DT$

Table 2 lists the values for these constants resident in Aspen Plus' databank.

Table 2. Values of constants for temperature-dependent expressions for the equilibrium constants from Aspen. [from aspen run on 1677 computer]

Parameter	A	B	C	D
Reaction 1	0	0	0	0
Reaction 2	-3.038325	-7008.356934	0	-0.003135
Reaction 3	216.050446	-12431.700195	-35.481899	0
Reaction 4	-0.52135	-2545.53	0	0
Reaction 5	-25.290564	1333.400024	0	0
Reaction 6	-5.978673	637.395996	0	-0.015134
Reaction 7	-9.4165	-4234.38	0	0
Reaction 8	-3.68672	-6754.686035	0	0
Reaction 9	231.465439	-12092.099609	-36.781601	0

Blocks and Streams

In this section we describe the blocks, or pieces of equipment, and list the values input into the model. We chose to use English units for the input values. Since we are comparing model results from the Huaneng Group in metric (SI) units and actual process values from Duke Energy expressed in English units, it is necessary to present the results in both systems. We did this by exporting the results to an Excel spreadsheet, converting the English to SI, and listing both. The blocks are listed in order of their appearance on the flow diagram.

The Aspen input data lists streams separately from blocks. However, in this description, we include the streams with the attached blocks for clarity. The Aspen Plus Input Summary for run number 212071020MW-4.2MolAmine.bkp is given in Appendix B.

Flue Gas Compressor (COMP)

This is a fan to increase the pressure of the flue gas, initially at atmospheric pressure, to overcome the resistance of the packed absorber column. We entered an outlet pressure of 0.4 psig (1.04 bar) for this block.

The input stream to this compressor is the flue gas stream (FLUEGAS) with the following input specifications:

- Temperature 130°F (44.4°C)
- Pressure 0 psig (1.01 bar)
- Molar flow rate (9.489 kmol/s)
- Mole flow of components
  - Carbon dioxide 7073.47 lbmol/h
  - Water 11533.5 lbmol/h
  - Nitrogen 50293.6 lbmol/h
  - Oxygen 4871.67 lbmol/h
  - Sulfur dioxide 1.476 lbmol/h
  - Hydrogen chloride 0.0667 lbmol/h

The output stream to the compressor is the stream COMPFLU. Aspen Plus calculates the properties of this stream.

Precooler (PRECOOL)

This is modeled as a "FLASH" block, a heat exchanger and separator to cool the incoming pressurized flue gas to a temperature that would result in improved absorption of the carbon dioxide by the amine solvent. We evaluated several outlet temperatures because of the tradeoff between CO_2 removal efficiency and cooling cost. We chose a temperature of 112°F (44.4°C) after the evaluation. At this temperature, approximately half of the water was removed in this block.

This block has one input stream and two output streams. The input stream, COMPFLU, comes from the compressor, COMP. Aspen calculates the liquid outlet stream, WATEROUT, to waste, and the vapor outlet stream, FEEDGAS, to the ABSORBER inlet.

Feed Mixer (FEEDMIX)

This block sets the liquid feed to the absorber column as a combination of the recycled stream from later in the process and a makeup stream containing the proper amount of water and amine to adjust the concentrations. Although Aspen has the ability to iterate a recycle loop until the makeup stream (AMINEFD) is converged, we chose to separate the recycle stream (REC) from the its counterpart (REC2) that goes into this block, adjust the AMINEFD stream, and rerun until steady state is achieved. The output from the FEEDMIX block, COMBFD, is the liquid feed to the top of the column, ABSORBER.

Absorber Column (ABSORBER)

The absorber column is modeled as a "RADFRAC" block. The absorber and the stripper, to be described later, are the main vehicles of the separation, and therefore require a large amount of specification information. The absorber contains plates or packing so that, as the amine solution flows downward in the column, it is in intimate contact with the CO_2-containing gas flowing upward. If the column contains packing instead of plates, the term "height equivalent to a theoretical plate" (HETP) is used to convert the number of plates to the height of the column. In the RADFRAC model, in each plate, the gas and liquid phases are assumed to be in equilibrium. Freguia,[21] Liu,[22] and others determined that the absorber column is rate controlled, so the equilibrium assumption will underestimate the number of plates required, and thus the height of the column. We used Freguia's estimates of HETP to estimate the column height because at the time we did not have Aspen's Rate Base Distillation.

We only briefly describe the design of an absorption or distillation column here, since entire graduate-level courses and textbooks are dedicated to this area. The reader is directed to any textbook on the subject for more information.

We set the following specifications for the absorber column. Many of these specifications were not set initially. For example, the number of plates was input initially, and, after several runs with different values, the final plate count was set. If the specified number of plates is too low, the desired separation cannot be achieved. If too many plates are specified, the equipment cost is higher than necessary. These are the specifications for the absorber:

- Column packing Koch Flexipac 2.5Y structured packing
- HETP 0.833 ft
- Number of plates 6
- COMBFD to plate 3
- FEEDGAS to plate 6, on-stage
- COND to plate 1
- CLEANGAS is the vapor leaving plate 1
- LIQUIDOUT is the rich solvent leaving plate 6
- Pressure of top plate 1 inch water gauge
- Pressure of plate 2 1 inch water gauge
- No condenser—there is a condenser, but it is specified as a separate piece of equipment (COND); see below
- No reboiler—this is an absorption, not a distillation column
- Request Aspen to calculate the packing diameter

The input streams to the ABSORBER block are FEEDGAS, COMBFD, and OUTWASH, all calculated by Aspen. OUTWASH will be described in the next section. The output streams are RICHOUT, the CO_2-rich liquid stream exiting the bottom of ABSORBER, and TOWASH, the vapor stream from the top of ABSORBER. Aspen calculates all of these streams.

Condenser (COND)

The condenser, modeled as a FLASH block, purifies the CO_2-free flue gas that exits the top of the absorber by cooling the gas to condense much of the water and amine in the stream. Also, a small amount of wash water (WASHWT) is added to improve the cleaning. The wash water and condensed water and amine flow back to the top of the absorber column. The specifications of the block, COND, are 1 atmosphere pressure and 142.7°F (61.5°C) The stream, CLEANER, is the flue gas with 90% of the CO_2 and some water removed. In our simulation, the condenser is operated at a higher temperature than the vapor exiting the column because the simulation results show that no water or amine reach this point. If, in practice, some carryover in the form of vapor or particulate is experienced, this temperature can be adjusted.

The input streams to COND are TOWASH, the vapor stream from ABSORBER, which is calculated by Aspen, and the wash water stream, WASHWT, which is specified by the user. We used 40 pounds per second (18 kg/s), one atmosphere, and 103°F (40°C) for this stream, but these parameters can be changed if necessary in the actual process. The amount of water in the makeup stream, AMINEFD, is adjusted based on the amount of water in this stream. The outlet streams from COND are the cleaned flue gas, CLEANER, and the liquid returned to the column, ABSORBER. Aspen calculates both of the outlet streams.

Rich Solution Pump (PUMP)

This pump increases the pressure of the rich solution to overcome the pressure resistance of the regenerative heat exchanger and to match the operating pressure of the regenerator column, which is higher than that of the absorber, which is operated close to atmospheric pressure. The pump specification is an outlet pressure of 49 psig (4.4 bar).

The input stream to this pump is RICHOUT, the rich solution from ABSORBER; the output stream, the cold inlet to the regenerative heat exchanger, REGEN, is RICHTOHX. Aspen calculates both streams.

Regenerative Heat Exchanger (REGEN) and Heat Exchanger (COOLER)

This heat exchanger cools a hot stream as it heats a cool stream without outside heat or cooling input. Since the heating and cooling energy are same, in heating the cold stream (RICHTOHX to STRIPFEE) to this temperature, the hot stream (LEANTOHX) is only cooled to 143.2°F (61.8°C), so an additional heat exchanger (COOLER) is necessary to cool this stream down to the amine feed temperature of 112°F (44.4°C).

The cold inlet and outlet streams are RICHOUT, described above, and STRIPFEE, the feed stream to the stripper column, STRIP. We specified the outlet temperature for the cold stream (STRIPFEE) at 205°F (96°C). Aspen calculates the hot inlet and outlet streams, LEANTOHX and LEANFRHX.

Stripper Column (STRIP)

This column, a RADFRAC block, is operated at higher temperature than the absorber column to reverse the reactions and release CO_2 from the amine solution. This column has a reboiler at the bottom to generate steam as it provides heat for the separation. The rich solution (STRIPFEE) is fed to the top of the column and exits as a hot, lean solution (LEANOUT) as the CO_2 and some water exits from the top of

the column, to be compressed and cooled to liquid CO_2 for sequestration. These are the specifications for the block STRIP:

- Column packing Koch Flexipac 2.5Y structured packing
- HETP 0.833 ft
- Number of plates 6
- COMBFD to plate 3
- REFFLUX to plate 1
- STRIPFEE to plate 1
- VAPOR is the vapor leaving plate 1
- LIQUID is the lean solvent leaving plate 6
- Pressure of top plate 1.5 atm absolute
- Pressure of plate 1.5 atm absolute
- No condenser—there is a condenser, but it is specified as a separate piece of equipment (DRYER); see below
- Reboiler is plate 6
- Request Aspen to calculate the packing diameter

The inlet streams to STRIP are STRIPFEE, described above, and REFLUX, from the condenser, DRYER, described below. Aspen calculates the REFLUX stream, the outlet stream, VAPOR, the high CO_2 vapor outlet to the condenser, DRYER, and LEANOUT, the CO_2-depleted solution to the recycle pump, RECYCLEP. Aspen calculates both outlet streams based on the specifications of STRIP.

Stripper Condenser (DRYER)

This condenser is a FLASH block that cools the outlet gas from the stripper and removes 90% of the water without reducing the CO_2 level. The specifications of this block are 117.9°F (47.7°C) and 7.35 psig (1.52 bar).

The inlet stream to DRYER is the vapor stream, VAPOR, from the column, STRIP, described above. Aspen calculates the outlet streams, REFLUX, liquid returning to the column, STRIP, and GASFSTR, vapor to CO_2 compression, based on the specifications of DRYER.

CO_2 Compressor (COMP1-COMP5 and COND1-COND5)

Although Aspen has a model for a multistage compressor with interstage cooling, we chose to model each compressor and cooler separately. We specified the compressor outlet pressures as 40, 125, 336, 868, and 2200 psig (3.82, 9.61, 24.2, 60.8, and 153 bar). We specified the output temperature of each condenser to be 112°F (44.4°C), consistent with Duke's maximum cooling-pond temperature of 104°F (40°C). Although the output stream from the final stage cooler is called CO2LIQ, this stream is 100% vapor because it is above the critical temperature of 87.89°F (31.05°C), so cannot be a liquid. Under these conditions, the vapor, before further cooling, has a specific volume of about 5 cubic meters per metric ton.

Aspen Process Model and Results

Appendix A contains the stream and equipment information calculated by Aspen. Appendix B contains the input file for the Aspen run described above, namely carbon capture using 35% by weight, mixed amines.

Appendix A. Results for Carbon Capture Using Mixed Amines at 35% by Weight

The results listed below are presented in English units only. Table A1 contains the stream data. Table A2 contains the remaining data that we used to evaluate the model. Figure A1 is the process flow diagram (PFD), and is the same as Figure 1 above. Tables A1.a through A1.d describe the streams from the PFD. In addition to the properties of each stream in the PFD, Aspen calculated the energy usages for each piece of equipment. The reader is directed to the Technoeconomic Evaluation for information on these energy usages.

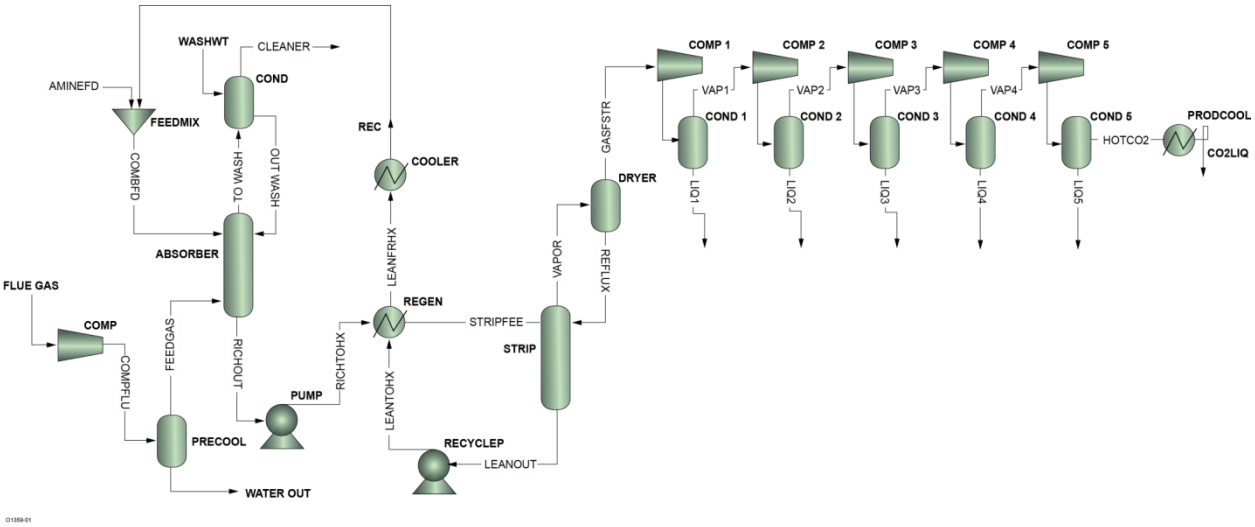


Table 1. Process flow diagram for carbon capture

Table A.1a. Stream Table: 35% Mixed Amine Solvent.

Stream Name	FLUEGAS	COMPFLU	WATEROUT	FEEDGAS	TOWASH	CLEANER
Temperature °C	54.4	55	44.4	44.4	51.5	51.2
Pressure, bar	1.011	1.037	1.037	1.037	1.016	1.014
Component Mole Flow, kmol/hr						
CO2	3,300	3,300	-	3,300	300	300
H2O	5,300	5,300	2,500	2,900	3,900	3,900
N2	23,000	23,000	-	23,000	23,000	23,000
O2	2,300	2,300	-	2,300	2,300	2,300
HCL	-	-	-	-	-	-
H3O+	-	-	-	-	-	-
HCO3-	-	-	-	-	-	-
CL-	-	-	-	-	-	-
CO3--	-	-	-	-	-	-
MEA	-	-	-	-	-	-
MEA+	-	-	-	-	-	-
MEACOO-	-	-	-	-	-	-
MDEA	-	-	-	-	-	-
AMP	-	-	-	-	-	-
AMP+	-	-	-	-	-	-
MDEA+	-	-	-	-	-	-
Component Mass Flow, kg/hr						
CO2	144,000	144,000	-	144,000	14,000	14,000
H2O	96,000	96,000	44,000	52,000	71,000	70,000
N2	652,000	652,000	-	652,000	652,000	652,000
O2	72,000	72,000	-	72,000	72,000	72,000
HCL	-	-	-	-	-	-
H3O+	-	-	-	-	-	-
HCO3-	-	-	-	-	-	-
CL-	-	-	-	-	-	-
CO3--	-	-	-	-	-	-
MEA	-	-	-	-	-	-
MEA+	-	-	-	-	-	-
MEACOO-	-	-	-	-	-	-
MDEA	-	-	-	-	-	-
AMP	-	-	-	-	-	-
AMP+	-	-	-	-	-	-
MDEA+	-	-	-	-	-	-
Total Flow, kmol/hr	34,000	34,000	2,500	32,000	30,000	30,000
Total Flow, kg/hr	965,000	965,000	44,000	921,000	810,000	809,000
Total Flow, cum/hr	914,000	896,000	43	806,000	792,000	790,000
Vapor Fraction	1	1	0	1	1	1
Liquid Fraction	0	0	1	0	0	0

Table A.1b. Stream Table: 35% Mixed Amine Solvent.

Stream Name	AMINEFD	REC	COMBFD	OUTWASH	RICHOUT
Temperature °C	44.4	44.4	44.4	51.2	49.9
Pressure, bar	1.013	1.048	1.016	1.014	1.016
Component Mole Flow, kmol/hr					
CO2	-	-	-	-	4
H2O	3,600	117,000	114,000	3,700	116,000
N2	-	-	-	-	-
O2	-	-	-	-	-
HCL	-	-	-	-	-
H3O+	-	-	-	-	-
HCO3-	-	60	50	-	1,000
CL-	-	-	-	-	-
CO3--	-	22	22	-	58
MEA	-	2,500	2,500	-	180
MEA+	-	2,800	2,800	-	3,200
MEACOO-	-	3,700	3,600	-	5,600
MDEA	-	3,300	3,300	-	1,200
AMP	-	620	630	-	80
AMP+	-	600	590	-	1,100
MDEA+	-	360	350	-	2,400
Component Mass Flow, kg/hr					
CO2	-	-	-	-	130
H2O	65,000	2,103,000	2,060,000	66,000	2,090,000
N2	-	-	-	-	11
O2	-	-	-	-	4
HCL	-	-	-	-	-
H3O+	-	-	-	-	-
HCO3-	-	3,500	3,300	-	62,000
CL-	-	-	-	-	-
CO3--	-	1,400	1,300	-	3,400
MEA	-	150,000	155,000	-	11,000
MEA+	-	175,000	173,000	-	197,000
MEACOO-	-	382,000	377,000	-	582,000
MDEA	-	392,000	393,000	-	148,000
AMP	-	55,000	56,000	-	7,300
AMP+	-	54,000	53,000	-	102,000
MDEA+	-	43,000	41,000	-	289,000
Total Flow, kmol/hr	3,600	131,000	128,000	3,700	131,000
Total Flow, kg/hr	65,000	3,359,000	3,313,000	66,000	3,491,000
Total Flow, cum/hr	65	3,400	3,400	68	3,500
Vapor Fraction	0	0	0	0	0
Liquid Fraction	1	1	1	1	1

Table A.1c. Stream Table: 35% Mixed Amine Solvent.

Stream Name	STRIPFEE	LEANOUT	VAPOR	REFLUX	GASFSTR	CO2LIQ
Temperature °C	99.5	111.0	98.1	47.7	47.7	44.4
Pressure, bar	1.662	1.52	1.52	1.52	1.52	153
Component Mole Flow, kmol/hr						
CO2	910	7	3,000	-	2,900	2,900
H2O	117,000	111,000	3,500	3,200	230	11
N2	-	-	-	-	-	-
O2	-	-	-	-	-	-
HCL	-	-	-	-	-	-
H3O+	-	-	-	-	-	-
HCO3-	500	170	-	-	-	-
CL-	-	-	-	-	-	-
CO3--	11	4	-	-	-	-
MEA	830	3,000	-	-	-	-
MEA+	2,900	2,400	-	-	-	-
MEACOO-	5,200	3,500	-	-	-	-
MDEA	1,700	2,800	-	-	-	-
AMP	290	730	-	-	-	-
AMP+	930	490	-	-	-	-
MDEA+	1,900	817	-	-	-	-
Component Mass Flow, kg/hr						
CO2	40,000	350	130,000	72	130,000	130,000
H2O	2,100,000	2,101,000	62,000	58,000	4,200	173
N2	11	-	11	-	11	11
O2	4	-	4	-	4	4
HCL	-	-	-	-	-	-
H3O+	-	-	-	-	-	-
HCO3-	33,000	11,000	-	97	-	-
CL-	-	-	-	-	-	-
CO3--	730	280	-	-	-	-
MEA	51,000	182,000	68	-	-	-
MEA+	181,000	150,000	-	68	-	-
MEACOO-	541,000	370,000	-	-	-	-
MDEA	207,000	336,000	44	-	-	-
AMP	26,000	64,000	11	-	-	-
AMP+	84,000	45,000	-	11	-	-
MDEA+	230,000	100,000	-	43	-	-
Total Flow, kmol/hr	132,000	131,000	6,400	3,200	3,200	3,000
Total Flow, kg/hr	3,492,000	3,359,000	191,000	59,000	133,000	130,000
Total Flow, cum/hr	38,000	3,600	129,000	58	55,000	190
Vapor Fraction	0.014	0	1	0	1	1
Liquid Fraction	0.986	1	0	1	0	0

Table A.1d. Stream Table: 35% Mixed Amine Solvent.

Stream Name	LEANTOHX	LEANFRHX	RICHTOHX
Temperature °C	111.3	54.5	50.1
Pressure, bar	1.703	1.703	442
Component Mole Flow, kmol/hr			
CO2	7	-	4
H2O	117,000	117,000	116,000
N2	-	-	-
O2	-	-	-
HCL	-	-	-
H3O+	-	-	-
HCO3-	180	72	1,000
CL-	-	-	-
CO3--	4	18	58
MEA	3,000	2,500	200
MEA+	2,400	2,700	3,200
MEACOO-	3,500	3,700	5,600
MDEA	2,800	3,200	1,200
AMP	720	630	83
AMP+	500	590	1,100
MDEA+	830	430	2,400
Component Mass Flow, kg/hr			
CO2	340	4	120
H2O	2,101,000	2,103,000	2,090,000
N2	-	-	11
O2	-	-	4
HCL	-	-	-
H3O+	-	-	-
HCO3-	11,000	4,000	62,000
CL-	-	-	-
CO3--	280	1080	3,400
MEA	182,000	155,000	11,000
MEA+	150,000	171,000	197,000
MEACOO-	370,000	381,000	582,000
MDEA	336,000	384,000	148,000
AMP	64,000	56,000	7,300
AMP+	45,000	53,000	102,000
MDEA+	100,000	52,000	290,000
Total Flow, kmol/hr	131,000	131,000	131,000
Total Flow, kg/hr	3,359,000	3,359,000	3,492,000
Total Flow, cum/hr	3,600	3,400	3,500
Vapor Fraction	0	0	0
Liquid Fraction	1	1	1

Appendix B. Aspen Input File for Mixed Amine Simulation

Following is the input file created by Aspen for run number 212071020MW-4.2MolAmine.bkp described in the main body.

```
;
;Input Summary created by Aspen Plus Rel. 26.0 at 13:54:36 Thu Dec 5, 2013
;Directory C:\Users\jones56\Desktop\CarbonCapture\For modeldesc mmeo  Filename
C:\Users\jones56\AppData\Local\Temp\~apdb31.txt
;



TITLE 'Recreation of Huaneng model'

IN-UNITS SI

DEF-STREAMS CONVEN ALL

DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.

   Property Method: None

   Flow basis for input: Mole

   Stream report composition: Mole flow
   "

DATABANKS 'APV732 ASPENPCD' / 'APV732 AQUEOUS' / 'APV732 SOLIDS' &
      / 'APV732 INORGANIC' / 'APV732 PURE22'

PROP-SOURCES 'APV732 ASPENPCD' / 'APV732 AQUEOUS' /  &
     'APV732 SOLIDS' / 'APV732 INORGANIC' / 'APV732 PURE22'
```

```
COMPONENTS
   CO2 CO2 /
   H2O H2O /
   N2 N2 /
   O2 O2 /
   HCL HCL /
   H3O+ H3O+ /
   HCO3- HCO3- /
   CL- CL- /
   CO3-- CO3-2 /
   MEA C2H7NO /
   MEA+ C2H8NO+ /
   MEACOO- C3H6NO3- /
   MDEA C5H13NO2 /
   AMP C4H11NO-1 /
   AMP+ C4H12NO+ /
   MDEA+ C5H14NO2+

HENRY-COMPS GLOBAL CO2 HCL O2 N2

CHEMISTRY GLOBAL
   STOIC 1 HCL -1 / H2O -1 / CL- 1 / H3O+ 1
   STOIC 2 H2O -1 / MDEA+ -1 / MDEA 1 / H3O+ 1
   STOIC 3 H2O -1 / MEACOO- -1 / MEA 1 / HCO3- 1
   STOIC 4 H2O -1 / MEA+ -1 / MEA 1 / H3O+ 1
   STOIC 5 H2O -1 / HCO3- -1 / CO3-- 1 / H3O+ 1
   STOIC 6 H2O -2 / CO2 -1 / HCO3- 1 / H3O+ 1
   STOIC 7 H2O -1 / AMP+ -1 / AMP 1 / H3O+ 1
   K-STOIC 2 A=-9.4165 B=-4234.97998 C=0 D=0
   K-STOIC 3 A=1.282562 B=-3456.18
   K-STOIC 4 A=0.7996 B=-8094.81 C=0 D=-0.00748
   K-STOIC 5 A=216.050446 B=-12431.700195 C=-35.481899 D=0
   K-STOIC 6 A=231.465439 B=-12092.099609 C=-36.781601 D=0
   K-STOIC 7 A=-3.68672 B=-6754.686035 C=0 D=0

FLOWSHEET
   BLOCK ABSORBER IN=COMBFD OUTWASH FEEDGAS OUT=TOWASH  &
      RICHOUT
   BLOCK COMP IN=FLUEGAS OUT=COMPFLU
   BLOCK STRIP IN=STRIPFEE REFLUX OUT=VAPOR LEANOUT
   BLOCK COOLER IN=LEANFRHX OUT=REC
```

```
  BLOCK RECYCLEP IN=LEANOUT OUT=LEANTOHX
  BLOCK REGEN IN=LEANTOHX RICHTOHX OUT=LEANFRHX STRIPFEE
  BLOCK DRYER IN=VAPOR OUT=GASFSTR REFLUX
  BLOCK FEEDMIX IN=AMINEFD REC2 OUT=COMBFD
  BLOCK COND IN=TOWASH WASHWT OUT=CLEANER OUTWASH
  BLOCK COMP1 IN=GASFSTR OUT=COMP1ST
  BLOCK COMP2 IN=VAP1 OUT=COMP2
  BLOCK COMP3 IN=VAP2 OUT=COMP3
  BLOCK COMP4 IN=VAP3 OUT=COMP4
  BLOCK COMP5 IN=VAP4 OUT=COMP5
  BLOCK COND1 IN=COMP1ST OUT=VAP1 LIQ1
  BLOCK COND2 IN=COMP2 OUT=VAP2 LIQ2
  BLOCK COND3 IN=COMP3 OUT=VAP3 LIQ3
  BLOCK COND4 IN=COMP4 OUT=VAP4 LIQ4
  BLOCK COND5 IN=COMP5 OUT=HOTCO2 LIQ5
  BLOCK PRODCOOL IN=HOTCO2 OUT=CO2LIQ
  BLOCK PUMP IN=RICHOUT OUT=RICHTOHX
  BLOCK PRECOOL IN=COMPFLU OUT=FEEDGAS WATEROUT

PROPERTIES ELECNRTL HENRY-COMPS=GLOBAL CHEMISTRY=GLOBAL  &
    TRUE-COMPS=YES

PROP-DATA HENRY-1
  IN-UNITS ENG PRESSURE=Pa TEMPERATURE=K PDROP=psi
  PROP-LIST HENRY
  BPVAL CO2 H2O 170.7126 -8477.711 -21.95743 .005780748 0.0  &
    2000.000 0.0
  BPVAL CO2 MEA 89.452 -2934.6 -11.592 0.01644 0.0 2000.000  &
    0.0
  BPVAL CO2 MDEA 89.452 -2934.6 -11.592 0.01644 0.0  &
    2000.000 0.0
  BPVAL CO2 AMP 89.452 -2934.6 -11.592 0.01644 0.0 2000.000  &
    0.0

PROP-DATA HENRY-1
  IN-UNITS ENG
  PROP-LIST HENRY
  BPVAL N2 H2O 180.3399883 -15178.98600 -21.55800000  &
    -4.6868000E-3 31.73000000 163.1300000 0.0
  BPVAL O2 H2O 157.8962298 -13995.10800 -18.39740000  &
    -5.2464111E-3 33.53000000 166.7300000 0.0
  BPVAL HCL H2O 49.61444341 -13973.09760 0.0 0.0 31.73000000  &
```

```
      260.3300000 0.0

PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL CO2 H2O 10.06400000 -5882.643000 .2000000000 0.0 0.0  &
      0.0 32.00000000 392.0000000
   BPVAL H2O CO2 10.06400000 -5882.643000 .2000000000 0.0 0.0  &
      0.0 32.00000000 392.0000000
   BPVAL H2O MEA 1.438498000 178.2378720 .2000000000 0.0 0.0  &
      0.0 77.00000000 302.0000000
   BPVAL MEA H2O -1.046602000 -607.5820800 .2000000000 0.0  &
      0.0 0.0 77.00000000 302.0000000

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H3O+ CL- .5534556901 .2140997379

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL CO2 ( H3O+ HCO3- ) 15.00000000
   PPVAL ( H3O+ HCO3- ) CO2 -8.000000000
   PPVAL CO2 ( H3O+ CO3-- ) 15.00000000
   PPVAL ( H3O+ CO3-- ) CO2 -8.000000000
   PPVAL H2O ( H3O+ HCO3- ) 8.045000000
   PPVAL ( H3O+ HCO3- ) H2O -4.072000000
   PPVAL H2O ( H3O+ CL- ) 4.110129000
   PPVAL ( H3O+ CL- ) H2O -3.344103000
   PPVAL H2O ( H3O+ CO3-- ) 8.045000000
   PPVAL ( H3O+ CO3-- ) H2O -4.072000000
   PPVAL HCL ( H3O+ CL- ) 12.00000000
   PPVAL ( H3O+ CL- ) HCL -1.0000000E-3
   PPVAL MEA ( H3O+ HCO3- ) 15.00000000
   PPVAL ( H3O+ HCO3- ) MEA -8.000000000
   PPVAL MEA ( H3O+ CO3-- ) 15.00000000
   PPVAL ( H3O+ CO3-- ) MEA -8.000000000
   PPVAL CO2 ( H3O+ MEACOO- ) 15.00000000
   PPVAL ( H3O+ MEACOO- ) CO2 -8.000000000
   PPVAL CO2 ( MEA+ HCO3- ) 15.00000000
   PPVAL ( MEA+ HCO3- ) CO2 -8.000000000
```

PPVAL CO2 (MEA+ CO3--) 15.00000000
PPVAL (MEA+ CO3--) CO2 -8.000000000
PPVAL CO2 (MEA+ MEACOO-) 15.00000000
PPVAL (MEA+ MEACOO-) CO2 -8.000000000
PPVAL H2O (MEA+ HCO3-) 6.885000
PPVAL (MEA+ HCO3-) H2O -3.899000
PPVAL H2O (MEA+ MEACOO-) 10.407000
PPVAL (MEA+ MEACOO-) H2O -5.963
PPVAL MEA (H3O+ MEACOO-) 15.00000000
PPVAL (H3O+ MEACOO-) MEA -8.000000000
PPVAL MEA (MEA+ HCO3-) 15.00000000
PPVAL (MEA+ HCO3-) MEA -8.000000000
PPVAL MEA (MEA+ CO3--) 15.00000000
PPVAL (MEA+ CO3--) MEA -8.000000000
PPVAL MEA (MEA+ MEACOO-) 15.00000000
PPVAL (MEA+ MEACOO-) MEA -8.000000000
PPVAL MDEA (H3O+ HCO3-) 15.00000000
PPVAL (H3O+ HCO3-) MDEA -8.000000000
PPVAL MDEA (H3O+ CO3--) 15.00000000
PPVAL (H3O+ CO3--) MDEA -8.000000000
PPVAL AMP (H3O+ HCO3-) 15.00000000
PPVAL (H3O+ HCO3-) AMP -8.000000000
PPVAL AMP (H3O+ CO3--) 15.00000000
PPVAL (H3O+ CO3--) AMP -8.000000000
PPVAL CO2 (AMP+ HCO3-) 15.00000000
PPVAL (AMP+ HCO3-) CO2 -8.000000000
PPVAL CO2 (AMP+ CO3--) 15.00000000
PPVAL (AMP+ CO3--) CO2 -8.000000000
PPVAL CO2 (MDEA+ HCO3-) 15.00000000
PPVAL (MDEA+ HCO3-) CO2 -8.000000000
PPVAL CO2 (MDEA+ CO3--) 15.00000000
PPVAL (MDEA+ CO3--) CO2 -8.000000000
PPVAL H2O (AMP+ HCO3-) 22.52879000
PPVAL (AMP+ HCO3-) H2O -11.30404000
PPVAL H2O (MDEA+ HCO3-) 26.16413000
PPVAL (MDEA+ HCO3-) H2O -14.35147000
PPVAL MDEA (MDEA+ HCO3-) 8.666588000
PPVAL (MDEA+ HCO3-) MDEA -5.804797000
PPVAL MDEA (MDEA+ CO3--) 15.00000000
PPVAL (MDEA+ CO3--) MDEA -8.000000000
PPVAL AMP (AMP+ HCO3-) 15.00000000
PPVAL (AMP+ HCO3-) AMP -8.000000000

```
    PPVAL AMP ( AMP+ CO3-- ) 15.00000000
    PPVAL ( AMP+ CO3-- ) AMP -8.000000000

PROP-DATA GMELCD-1
    IN-UNITS ENG
    PROP-LIST GMELCD
    PPVAL CO2 ( H3O+ HCO3- ) 0.0
    PPVAL ( H3O+ HCO3- ) CO2 0.0
    PPVAL CO2 ( H3O+ CO3-- ) 0.0
    PPVAL ( H3O+ CO3-- ) CO2 0.0
    PPVAL H2O ( H3O+ CL- ) 4151.955600
    PPVAL ( H3O+ CL- ) H2O -1176.370380
    PPVAL HCL ( H3O+ CL- ) 0.0
    PPVAL ( H3O+ CL- ) HCL 0.0
    PPVAL MEA ( H3O+ HCO3- ) 0.0
    PPVAL ( H3O+ HCO3- ) MEA 0.0
    PPVAL MEA ( H3O+ CO3-- ) 0.0
    PPVAL ( H3O+ CO3-- ) MEA 0.0
    PPVAL CO2 ( H3O+ MEACOO- ) 0.0
    PPVAL ( H3O+ MEACOO- ) CO2 0.0
    PPVAL CO2 ( MEA+ HCO3- ) 0.0
    PPVAL ( MEA+ HCO3- ) CO2 0.0
    PPVAL CO2 ( MEA+ CO3-- ) 0.0
    PPVAL ( MEA+ CO3-- ) CO2 0.0
    PPVAL CO2 ( MEA+ MEACOO- ) 0.0
    PPVAL ( MEA+ MEACOO- ) CO2 0.0
    PPVAL H2O ( MEA+ HCO3- ) 969.636
    PPVAL ( MEA+ HCO3- ) H2O -91.347
    PPVAL H2O ( MEA+ MEACOO- ) -119.927
    PPVAL ( MEA+ MEACOO- ) H2O 336.452
    PPVAL MEA ( H3O+ MEACOO- ) 0.0
    PPVAL ( H3O+ MEACOO- ) MEA 0.0
    PPVAL MEA ( MEA+ HCO3- ) 0.0
    PPVAL ( MEA+ HCO3- ) MEA 0.0
    PPVAL MEA ( MEA+ CO3-- ) 0.0
    PPVAL ( MEA+ CO3-- ) MEA 0.0
    PPVAL MEA ( MEA+ MEACOO- ) 0.0
    PPVAL ( MEA+ MEACOO- ) MEA 0.0
    PPVAL MDEA ( H3O+ HCO3- ) 0.0
    PPVAL ( H3O+ HCO3- ) MDEA 0.0
    PPVAL MDEA ( H3O+ CO3-- ) 0.0
    PPVAL ( H3O+ CO3-- ) MDEA 0.0
```

PPVAL AMP (H3O+ HCO3-) 0.0
PPVAL (H3O+ HCO3-) AMP 0.0
PPVAL AMP (H3O+ CO3--) 0.0
PPVAL (H3O+ CO3--) AMP 0.0
PPVAL CO2 (AMP+ HCO3-) 0.0
PPVAL (AMP+ HCO3-) CO2 0.0
PPVAL CO2 (AMP+ CO3--) 0.0
PPVAL (AMP+ CO3--) CO2 0.0
PPVAL CO2 (MDEA+ HCO3-) 0.0
PPVAL (MDEA+ HCO3-) CO2 0.0
PPVAL CO2 (MDEA+ CO3--) 0.0
PPVAL (MDEA+ CO3--) CO2 0.0
PPVAL H2O (AMP+ HCO3-) -7738.117200
PPVAL (AMP+ HCO3-) H2O 4051.369800
PPVAL H2O (MDEA+ HCO3-) -11966.33340
PPVAL (MDEA+ HCO3-) H2O 6865.635600
PPVAL MDEA (MDEA+ HCO3-) 0.0
PPVAL (MDEA+ HCO3-) MDEA 0.0
PPVAL MDEA (MDEA+ CO3--) 0.0
PPVAL (MDEA+ CO3--) MDEA 0.0
PPVAL AMP (AMP+ HCO3-) 0.0
PPVAL (AMP+ HCO3-) AMP 0.0
PPVAL AMP (AMP+ CO3--) 0.0
PPVAL (AMP+ CO3--) AMP 0.0

PROP-DATA GMELCE-1
IN-UNITS ENG
PROP-LIST GMELCE
PPVAL CO2 (H3O+ HCO3-) 0.0
PPVAL (H3O+ HCO3-) CO2 0.0
PPVAL CO2 (H3O+ CO3--) 0.0
PPVAL (H3O+ CO3--) CO2 0.0
PPVAL H2O (H3O+ CL-) .3417959000
PPVAL (H3O+ CL-) H2O 2.121453000
PPVAL HCL (H3O+ CL-) 0.0
PPVAL (H3O+ CL-) HCL 0.0
PPVAL MEA (H3O+ HCO3-) 0.0
PPVAL (H3O+ HCO3-) MEA 0.0
PPVAL MEA (H3O+ CO3--) 0.0
PPVAL (H3O+ CO3--) MEA 0.0
PPVAL CO2 (H3O+ MEACOO-) 0.0
PPVAL (H3O+ MEACOO-) CO2 0.0

```
    PPVAL CO2 ( MEA+ HCO3- ) 0.0
    PPVAL ( MEA+ HCO3- ) CO2 0.0
    PPVAL CO2 ( MEA+ CO3-- ) 0.0
    PPVAL ( MEA+ CO3-- ) CO2 0.0
    PPVAL CO2 ( MEA+ MEACOO- ) 0.0
    PPVAL ( MEA+ MEACOO- ) CO2 0.0
    PPVAL MEA ( H3O+ MEACOO- ) 0.0
    PPVAL ( H3O+ MEACOO- ) MEA 0.0
    PPVAL MEA ( MEA+ HCO3- ) 0.0
    PPVAL ( MEA+ HCO3- ) MEA 0.0
    PPVAL MEA ( MEA+ CO3-- ) 0.0
    PPVAL ( MEA+ CO3-- ) MEA 0.0
    PPVAL MEA ( MEA+ MEACOO- ) 0.0
    PPVAL ( MEA+ MEACOO- ) MEA 0.0
    PPVAL MDEA ( H3O+ HCO3- ) 0.0
    PPVAL ( H3O+ HCO3- ) MDEA 0.0
    PPVAL MDEA ( H3O+ CO3-- ) 0.0
    PPVAL ( H3O+ CO3-- ) MDEA 0.0
    PPVAL AMP ( H3O+ HCO3- ) 0.0
    PPVAL ( H3O+ HCO3- ) AMP 0.0
    PPVAL AMP ( H3O+ CO3-- ) 0.0
    PPVAL ( H3O+ CO3-- ) AMP 0.0
    PPVAL CO2 ( AMP+ HCO3- ) 0.0
    PPVAL ( AMP+ HCO3- ) CO2 0.0
    PPVAL CO2 ( AMP+ CO3-- ) 0.0
    PPVAL ( AMP+ CO3-- ) CO2 0.0
    PPVAL CO2 ( MDEA+ HCO3- ) 0.0
    PPVAL ( MDEA+ HCO3- ) CO2 0.0
    PPVAL CO2 ( MDEA+ CO3-- ) 0.0
    PPVAL ( MDEA+ CO3-- ) CO2 0.0
    PPVAL MDEA ( MDEA+ HCO3- ) 0.0
    PPVAL ( MDEA+ HCO3- ) MDEA 0.0
    PPVAL MDEA ( MDEA+ CO3-- ) 0.0
    PPVAL ( MDEA+ CO3-- ) MDEA 0.0
    PPVAL AMP ( AMP+ HCO3- ) 0.0
    PPVAL ( AMP+ HCO3- ) AMP 0.0
    PPVAL AMP ( AMP+ CO3-- ) 0.0
    PPVAL ( AMP+ CO3-- ) AMP 0.0

PROP-DATA GMELCN-1
    IN-UNITS ENG
    PROP-LIST GMELCN
```

```
   PPVAL CO2 ( H3O+ HCO3- ) .1000000000
   PPVAL CO2 ( H3O+ CO3-- ) .1000000000
   PPVAL MEA ( H3O+ HCO3- ) .1000000000
   PPVAL MEA ( H3O+ CO3-- ) .1000000000
   PPVAL CO2 ( H3O+ MEACOO- ) .1000000000
   PPVAL CO2 ( MEA+ HCO3- ) .1000000000
   PPVAL CO2 ( MEA+ CO3-- ) .1000000000
   PPVAL CO2 ( MEA+ MEACOO- ) .1000000000
   PPVAL MEA ( H3O+ MEACOO- ) .1000000000
   PPVAL MEA ( MEA+ HCO3- ) .1000000000
   PPVAL MEA ( MEA+ CO3-- ) .1000000000
   PPVAL MEA ( MEA+ MEACOO- ) .1000000000
   PPVAL MDEA ( H3O+ HCO3- ) .1000000000
   PPVAL MDEA ( H3O+ CO3-- ) .1000000000
   PPVAL AMP ( H3O+ HCO3- ) .1000000000
   PPVAL AMP ( H3O+ CO3-- ) .1000000000
   PPVAL CO2 ( AMP+ HCO3- ) .1000000000
   PPVAL CO2 ( AMP+ CO3-- ) .1000000000
   PPVAL CO2 ( MDEA+ HCO3- ) .1000000000
   PPVAL CO2 ( MDEA+ CO3-- ) .1000000000
   PPVAL MDEA ( MDEA+ HCO3- ) .1000000000
   PPVAL MDEA ( MDEA+ CO3-- ) .1000000000
   PPVAL AMP ( AMP+ HCO3- ) .1000000000
   PPVAL AMP ( AMP+ CO3-- ) .1000000000

STREAM AMINEFD
   SUBSTREAM MIXED TEMP=317.5944444 PRES=1.01281000E+5
   MOLE-FLOW H2O 1. / N2 0. / O2 0. / HCL 0. / H3O+  &
      0.

STREAM FLUEGAS
   SUBSTREAM MIXED TEMP=327.5944444 PRES=1.01101000E+5
   MOLE-FLOW CO2 0.909752 / H2O 1.483446 / N2 6.469231 /  &
      O2 0.626316 / HCL 0. / HCO3- 0.

STREAM REC2
   SUBSTREAM MIXED TEMP=317.5500000 PRES=1.01281000E+5
   MOLE-FLOW CO2 6.6128E-006 / H2O 30.767 / N2 0. / O2  &
      0. / HCL 0. / H3O+ 2.97E-010 / HCO3- 0.014 / CL-  &
      0. / CO3-- 0.006 / MEA 0.707 / MEA+ 0.772 /  &
      MEACOO- 1.007 / MDEA 0.916 / AMP 0.174 / AMP+  &
      0.164 / MDEA+ 0.097
```

```
STREAM WASHWT
   SUBSTREAM MIXED TEMP=40. <C> PRES=101.101 <kPa>
   MOLE-FLOW H2O 1.

BLOCK FEEDMIX MIXER
   PARAM PRES=1.01574089E+5

BLOCK COOLER HEATER
   PARAM TEMP=317.5500000 PRES=1.04791692E+6

BLOCK PRODCOOL HEATER
   PARAM TEMP=317.5500000 PRES=1.52718874E+7

BLOCK COND FLASH2
   PARAM PRES=1.01352932E+5 DUTY=0.0

BLOCK COND1 FLASH2
   PARAM TEMP=317.5944444 PRES=3.82659030E+5

BLOCK COND2 FLASH2
   PARAM TEMP=317.5944444 PRES=9.61818642E+5

BLOCK COND3 FLASH2
   PARAM TEMP=317.5944444 PRES=2.41800000E+6

BLOCK COND4 FLASH2
   PARAM TEMP=317.5944444 PRES=6.08255488E+6

BLOCK COND5 FLASH2
   PARAM TEMP=317.5944444 PRES=1.52718874E+7

BLOCK DRYER FLASH2
   PARAM TEMP=320.9277778 PRES=1.51987500E+5

BLOCK PRECOOL FLASH2
   PARAM TEMP=112. <F> PRES=103.681 <kPa>

BLOCK REGEN HEATX
   PARAM DELT-HOT=8. <F> CALC-TYPE=DESIGN  &
      PRES-COLD=1.66173000E+5 MIN-TAPP=4.444444444  &
      U-OPTION=PHASE F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
```

```
   FEEDS HOT=LEANTOHX COLD=RICHTOHX
   PRODUCTS HOT=LEANFRHX COLD=STRIPFEE
   HOT-SIDE DP-OPTION=CONSTANT
   COLD-SIDE DP-OPTION=CONSTANT

BLOCK ABSORBER RADFRAC
   PARAM NSTAGE=15 MAXOL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   RATESEP-ENAB CALC-MODE=EQUILIBRIUM
   PROP-SECTION 1 15 ELECNRTL HENRY-COMPS=GLOBAL  &
      CHEMISTRY=GLOBAL
   FEEDS COMBFD 3 / OUTWASH 1 / FEEDGAS 15 ON-STAGE
   PRODUCTS TOWASH 1 V / RICHOUT 15 L
   P-SPEC 1 1.01574089E+5 / 2 1.01574089E+5
   COL-SPECS
   HEATERS 4 -2.0000000E+7
   REAC-STAGES 1 15 GLOBAL
   PACK-SIZE 1 2 6 FLEXIPAC VENDOR=KOCH PACK-MAT=METAL  &
      PACK-SIZE="2.5Y" HETP=.2538984000 P-UPDATE=NO

BLOCK STRIP RADFRAC
   PARAM NSTAGE=6 ABSORBER=YES MAXOL=90 DAMPING=MILD
   COL-CONFIG CONDENSER=NONE REBOILER=KETTLE
   FEEDS STRIPFEE 1 ON-STAGE / REFLUX 1
   PRODUCTS VAPOR 1 V / LEANOUT 6 L
   P-SPEC 1 1.51987500E+5 / 2 1.51987500E+5
   COL-SPECS QN=1.09000000E+8
   REAC-STAGES 1 6 GLOBAL
   PACK-SIZE 1 1 5 FLEXIPAC VENDOR=KOCH PACK-MAT=METAL  &
      PACK-SIZE="2.5Y" HETP=.2538984000 P-UPDATE=NO

BLOCK PUMP PUMP
   PARAM PRES=4.41777000E+5

BLOCK RECYCLEP PUMP
   PARAM PRES=1.70272573E+5

BLOCK COMP COMPR
   PARAM TYPE=ISENTROPIC PRES=1.03681000E+5 SEFF=1. NPHASE=2
   BLOCK-OPTION FREE-WATER=NO

BLOCK COMP1 COMPR
```

```
   PARAM TYPE=ISENTROPIC PRES=3.82659030E+5 SEFF=0.92

BLOCK COMP2 COMPR
   PARAM TYPE=ISENTROPIC PRES=9.61818642E+5 SEFF=0.92 NPHASE=1
   BLOCK-OPTION FREE-WATER=NO

BLOCK COMP3 COMPR
   PARAM TYPE=ISENTROPIC PRES=2.41800000E+6 SEFF=0.92

BLOCK COMP4 COMPR
   PARAM TYPE=ISENTROPIC PRES=6.08186541E+6 SEFF=0.92 NPHASE=2
   BLOCK-OPTION FREE-WATER=NO

BLOCK COMP5 COMPR
   PARAM TYPE=ISENTROPIC PRES=15271887. SEFF=0.92 NPHASE=2
   BLOCK-OPTION FREE-WATER=NO

EO-CONV-OPTI

CALCULATOR WATF
   IN-UNITS ENG
   DEFINE WATF MOLE-FLOW STREAM=AMINEFD SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE AMFEE MOLE-FLOW STREAM=AMINEFD SUBSTREAM=MIXED  &
      COMPONENT=MEA
   DEFINE WATREC MOLE-FLOW STREAM=REC SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE AMREC MOLE-FLOW STREAM=REC SUBSTREAM=MIXED  &
      COMPONENT=MEA
F     WATFEE=455000-WATREC
F     AMFEE=45000-AMREC
   EXECUTE FIRST

CONV-OPTIONS
   WEGSTEIN MAXIT=10

STREAM-REPOR MOLEFLOW MASSFLOW

PROPERTY-REP NOPARAM-PLUS

DISABLE
   CALCULATOR WATF
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Appendix C. References

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