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ABSTRACT

This report discusses the replacement of water by carbon dioxide in both the quench stream and the supercritical water oxidation (SCWO) reactor feed in order to reduce the energy utilization in the process. FLUENT was used to generate the input requirements and ASPEN PLUS was used to model the SCWO process. Simulations were made for normal MODAR operating conditions (baseline case) and two other cases replacing water by carbon dioxide. The basis for and assumptions used in the simulation are given.

Economic evaluations were made and costs were compared with the baseline case and a case with 60% replacement of water by carbon dioxide. The equipment cost is almost the same. However, the case with replacement of water by carbon dioxide reduces the energy requirement in the end process by a factor of three, which is a significant energy savings in the operation.

Also, the injection of carbon dioxide into the SCWO reactor feed is expected to reduce corrosion and makes salt particles non-sticky. However, these advantages need to be confirmed by experiment.

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FIGURES

ALTERNATE FLUID TO IMPROVE ENERGY EFFICIENCY OF SUPERCRITICAL WATER OXIDATION PROCESS

1. INTRODUCTION

Because supercritical water has unique characteristic which makes organics miscible in it, water at supercritical conditions (Tc=374^{0}C, Pc=218 atm) is used as a solvent for mixing, a heat transfer media for preheating, a heat sink to control the fluid temperature, and a coolant to quench the reactor effluents in the supercritical water oxidation process. The extensive use of water to quench the effluent stream process results in very high energy requirements when separating this stream at the end process unit because water has a high heat of vaporization. We propose to replace as much of the water stream as possible by an alternate fluid which has heat transfer characteristics similar to those of water but which can be more economically separated from the hazardous or mixed wastes streams.

The MODAR process uses quench water flowrates that are 1.6 times the reactor effluent flowrate to quench the effluent to less than 300^{0}C before the first separator. This massive amount of water used in the quench stream goes into the end process unit where the water must be processed to separate wastes from the water. Preliminary ASPEN PLUS calculations indicate that carbon dioxide, one of the alternate fluid candidates, can be used to replace most of the quench water stream while adequately cooling the reactor effluents. It is recycled from the first separator, and is easily separately as a gas from the ppm level impurities in the end process.

This replacement results in significant water reduction in the end process, which reduces the energy duty by a factor of 3 in the end process unit and makes the supercritical water oxidation (SCWO) technology more economically viable. In addition, the replacement of water in the reactor feed by carbon dioxide would alleviate much of the sticky salt deposit problem because the salts remain in a solid form in the carbon dioxide environment due to the lower solubility of salt in carbon dioxide. In the water environment some salts remain sticky. Also, the higher viscosity of carbon dioxide at the supercritical conditions would minimize the corrosion problem because of the lower mass transfer rate of heteroatoms (e.g.,chlorine, sulphur, etc.) to the wall.

2. THE CURRENT SCWO PROCESS

There are three SCWO reactor configurations: tubular reactor, vertical vessel reactor, and transpiring platelet reactor, a porous wall reactor concept. The flow mixing is strongly coupled with the chemical kinetics and affects the destruction efficiency.[1,2] Therefore the flow mixing is very important and is dependant on the reactor geometry and the mixing device of the waste stream and air stream. The brief generic descriptions of the reactor concepts are summarized below.

2.1 Vertical Vessel Reactor

The vertical reactor concept consists of a co-axial nozzle for the feed stream, a brine pool in the lower conical section to separate salts, a cylindrical space for the oxidation and an outlet pipe in the upper section. The unique design characteristics of this configuration provide a brine pool to separate salts at the bottom of the reactor and the reaction effluents are removed through the pipe located in the upper section. Due to the flow exit at the upper section, the flow generates a recirculation pattern downstream of the nozzle. The flow entrainment caused by this recirculation provides a backmixing which preheats the incoming waste stream. Also, the nozzle design is very important for the reactant mixing and salt precipitation behavior.

2.2 Transpiring Platelet Reactor

This configuration is very similar to a straight tubular reactor, but it has a porous liner along the tube wall. Supercritical water and/or oxidants are injected radially into the axial waste flow to protect the wall from thermal stress, corrosion, and salt deposition on the wall surface. The reactor configuration consists of three sections: a preheating section, a reaction section, and a cooldown section. In the preheating section, hot water is injected through the porous wall to preheat the waste stream and to provide a boundary layer to protect the wall from corrosion expected at 400^0C, which is the mixing temperature in the preheating section. In the reaction section, hot air and supercritical water (SCW) are flowed through the porous wall while cold water is injected through the cooldown section porous wall to cool down the reaction effluent. In these regions, the amount of water injected through the porous wall must be processed in the end unit, which is an evaporator or ion exchange column.

2.3 Tubular Reactor

The simplest design of a SCWO reactor is a thin tubular pipe whose heated initial length serves as a preacher to bring the high pressure feeds to temperatures above the critical point of water. The oxidation then begins in the section in the mid portion of the reactor, in which the reactants are heated by the exothermic heat release to temperatures above the critical temperature and the reaction rate increases. Because the flow is plug flow, there is no radial mixing to promote flow mixing. As a result, this configuration requires a lengthy pipe. Since the reactor is long with a small diameter, salt precipitation on the reactor wall is a plaguing problem, because it can cause plug up the reactor.

2.4 MODAR Flow Process

Figure 1 shows a schematic of a typical MODAR pilot scale flow sheet. Air and water are fed through a heat exchanger into the reactor via the outer nozzle and waste and water via the inner nozzle. If the reaction generates acids, a neutralizing chemical such as NaCl is added to the waste stream stoichiometrically. The oxidation reaction occurs downstream of the nozzle, generating reaction products such as carbon dioxide and water. Heteroatoms are converted into inorganic compounds, usually acids, salts or oxides. Sulfur, if present in the feed stream, is converted into sulfate, phosphorus to phosphate, and halogens to haloacids. The reaction products, carbon dioxide and water, exit at the upper portion of the reactor and are filtered before they go to a heat exchanger to cool down. After they flow through another cooler, they enter the first separator, a medium pressure separator (1500 psia), where gases are removed at the top and liquids are fed into the second separator, a low pressure separator (100 psia), where the gas and liquid are removed at the top and bottom, respectively. If the liquid is still contaminated, it is recycled back to the reactor. If this occurs, it will reduce the waste treatment capacity. In chemical plants, the contaminated stream is treated in an ion-exchange column and/or evaporator. Precipitated salts are dissolved in the brine pool and removed at the bottom of the reactor. Then, the brine is separated at a third separator, a medium pressure separator (1450 psia).

Regardless of reactor types used in the SCWO process, the flow process is very similar to Figure 1 and requires a quenching system. In the vertical vessel reactor and tubular reactor, the quench stream is mixed with the reactor effluent stream, while the transpiring platelet reactor uses radial mixing in the reactor through the porous wall.

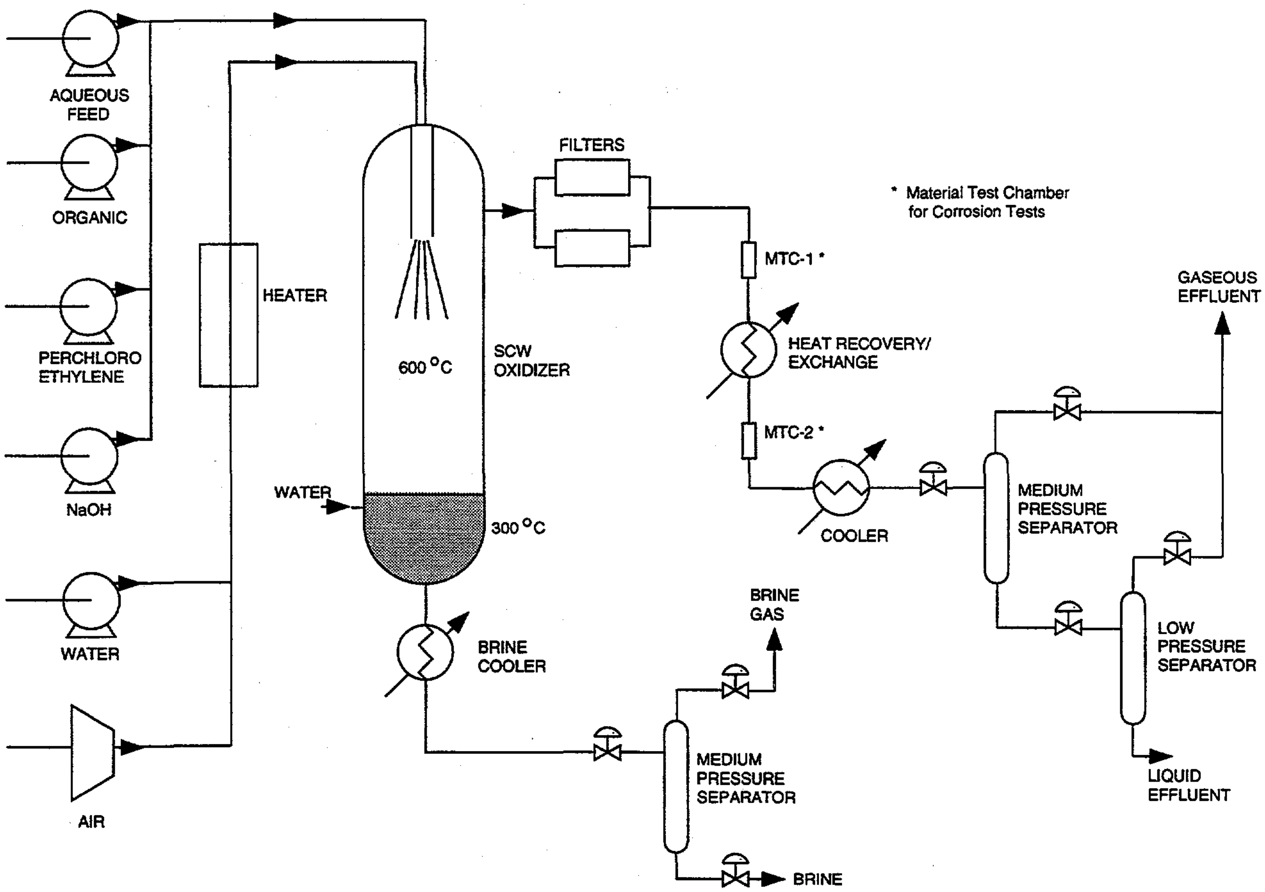

Figure 1. Modar's SCWO flow sheet

3. ENTHALPY CALCULATION AND PROPERTIES

3.1 Adiabatic Reaction Temperatures

We developed a method to calculate the adiabatic reaction temperature so it could be used to estimate the reactor temperature as a function of flows and temperatures of the input streams; this was determined to be very helpful in establishing sensitivities of reactor temperature to flow parameters and fluid properties.[3,4,5,6]

The adiabatic reaction temperature is defined as the temperature that would be reached if the fuel and oxidant streams mixed and reacted adiabatically. If the heat losses from the reactor are low, as they are in this pilot scale reactor, the steady state (mixed) outlet temperatures predicted by FLUENT[7] will converge to a value very near the theoretical adiabatic reaction temperature.

FLUENT solves the energy equation in terms of conservation of the static enthalpy, h, defined as:

$$h = \sum_i m_i \, h_i$$

where

$$h_i = \int_{T_{ref}}^{T} c_{p,\,i} \, dT$$

where m_i is the mass fraction, T_{ref} is a reference temperature (300 K in these calculations) and $c_{p,i}$ is the specific heat at constant pressure of species i. This sensible enthalpy does not include the enthalpy of formation of each species. For chemically reacting flows FLUENT calculates the instantaneous enthalpy, h^*, as:

$$\begin{aligned} h^* &= \sum_i m_i \left[\int_{T_{ref}}^{T} c_{p,\,i} \, dT + \frac{h_i^o}{M_i} + \int_{T_{ref_i}}^{T_{ref}} c_{p,\,i} \, dT \right] \\ &= \sum_i m_i \left[\int_{T_{ref_i}}^{T} c_{p,\,i} dT + \frac{h_i^o}{M_i} \right] \end{aligned}$$

where h_i^o is the enthalpy of formation of species i obtained at reference temperature T_{ref_i} (298.15 K in these calculations, see enthalpy of formation in 3.2.1), and M_i is the molecular weight of species i. FLUENT calculates and lists the values of h* for each cell in the computational domain using the temperatures, compositions, and properties available to it.

We calculate the adiabatic reaction temperature by mixing the instantaneous enthalpies of the core flow and the annular flow (fuel and oxidant, respectively) to obtain a mass averaged instantaneous enthalpy which, in the FLUENT representation, includes the heat of reaction, i. e.,

$$h^*_{mixed} = \frac{h^*_{core}\dot{m}_{core} + h^*_{annulus}\dot{m}_{annulus}}{\dot{m}_{core} + \dot{m}_{annulus}}$$

where $\dot{m}$ is the mass flow rate of the *core* and *annulus*.

FLUENT calculates the enthalpy at the core and annulus inlets based upon the model input conditions. Then, using complete oxidation compositions, a temperature is found by trial and error which results in the same mixed enthalpy as calculated above. This is the adiabatic reaction temperature. Using FLUENT to perform the enthalpy calculations we were able to ensure that the properties used and the calculation method matched those in the actual FLUENT runs. Inherent in this calculational method is the assumption of negligible heat transfer from the reaction zone. This is a good assumption because the reactor is well insulated in the upper regions of the reactor bounding the reaction zone. Also, since the lower region has very low flows, there is poor heat transfer between the hot reaction zone and the cold brine region.

Table 1 shows the results of our calculations of hot stream inlet temperatures as a function of both the core (inner nozzle) and annulus (outer nozzle) stream flowrates in order to achieve the adiabatic fluid temperature at 600^0C. This calculation was iterative assuming the inlet stream temperature and achieving the adiabatic temperature at 600^0C. An IPA flowrate of 165 lb/hr was used for all the calculations.

Table 1. Adiabatic reaction temperature

Case	Feed rate to nozzle (lb/hr)	Hot stream inlet temperature (F)
Baseline	3155 H_2O	1112
Case-A	2585 H_2O and 571 CO_2 (40% replacement)	930
Case-B	2869 H_2O and 286 CO_2 (20% replacement)	1012

3.2 Enthalpies of Formation

The formation enthalpies for all species entering into the chemical reactions, together with the reference temperatures at which these are defined, are required in the FLUENT model. The values used in these calculations were obtained from Reference 8 and are shown in Table 2.

Table 2. Enthalpies of formation for SCWO species.

	Formation enthalpy (J/kmol)	Reference temperature (K)
C_3H_8O	-3.11E08	298.15
H_2O	-2.85E08	298.15
CO_2	-3.94E08	298.15
O_2	0	298.15
N_2	0	298.15

In the above table the formation enthalpies of IPA and water were taken to be those of the liquid state, while that of CO_2 was taken to be a gas, representing their initial states.

3.3 Thermodynamic and Transport Properties

The critical point of water is at 3206 psia (22.1 MPa) and 374°C. A SCWO reactor is typically run at a pressure somewhat higher than the critical pressure; the reactor simulated in this report was operated at a constant pressure of 3500 psia (23.8 MPa).

The five chemical species considered in this application include IPA, water, carbon dioxide, oxygen, and nitrogen. Properties needed for the calculations include the specie densities, specific heats, viscosities, and thermal conductivities. These properties were obtained from the Aspen code[9] as a function of temperature for the range of 300 K to 1500 K and a constant pressure of 3400 psia. The vessel reactor has a relatively low pressure drop so the approximation of constant pressure properties will not introduce a significant error into the calculations. Water properties were calculated using the NBS correlations in the Aspen code, while the properties of the other fluids were calculated with the SR-Polar option.

Figure 2 through Figure 5 show the specific heat, density, viscosity, and thermal conductivity of all the species used in this study and also those of ethanol (ethanol was used in the bench scale study in Reference 5).

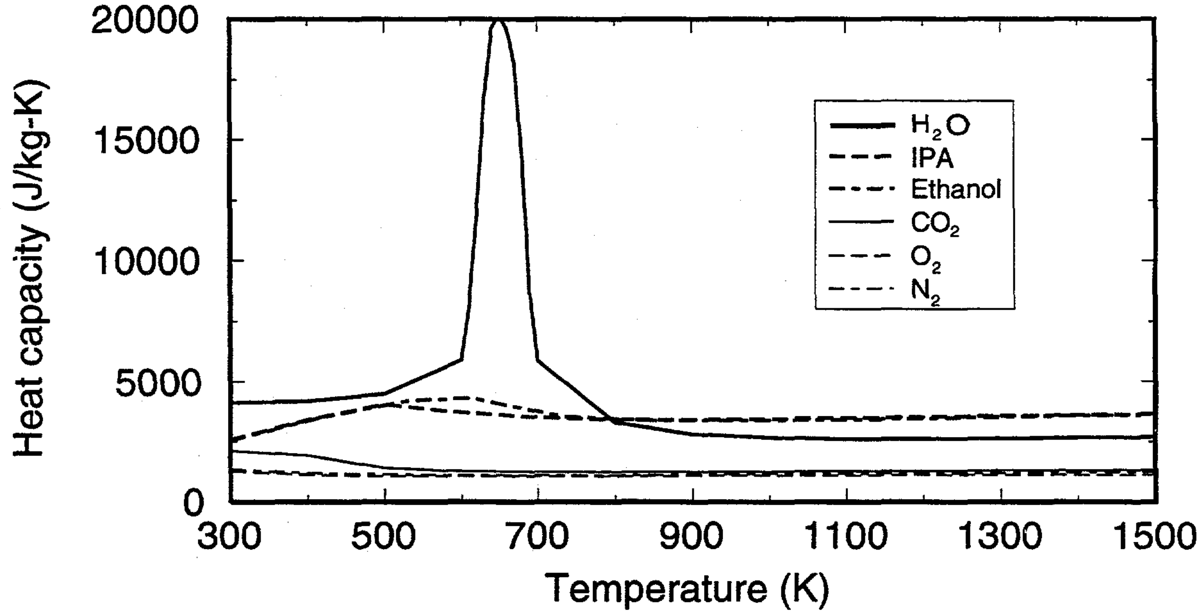

Figure 2. Specific heats of SCWO fluids.

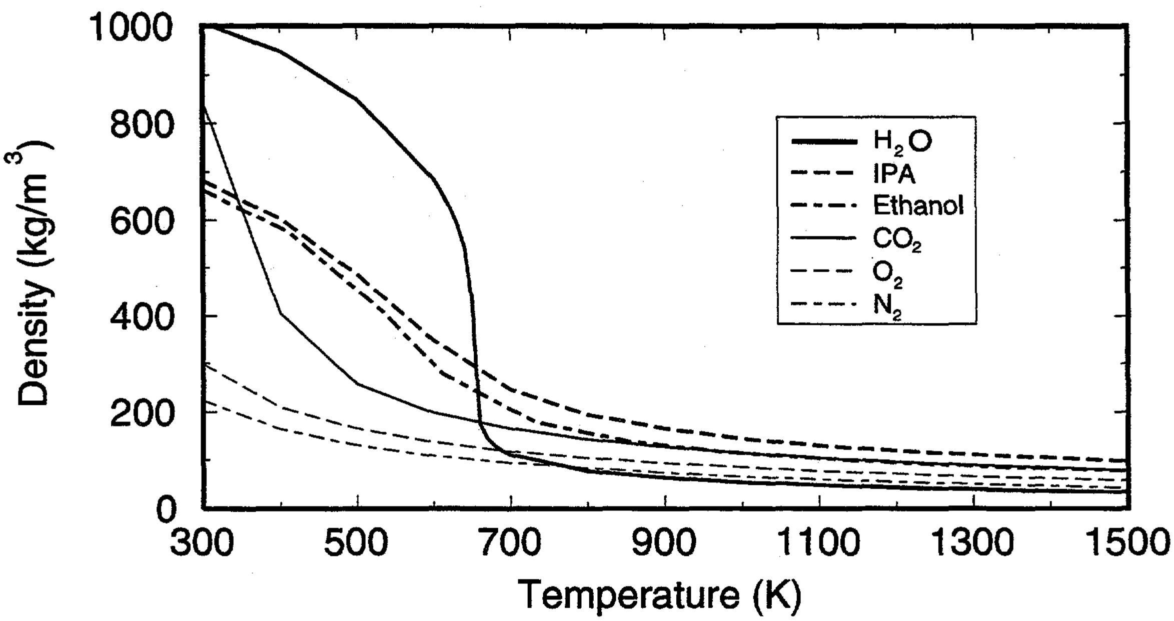

Figure 3. Densities of SCWO fluids.

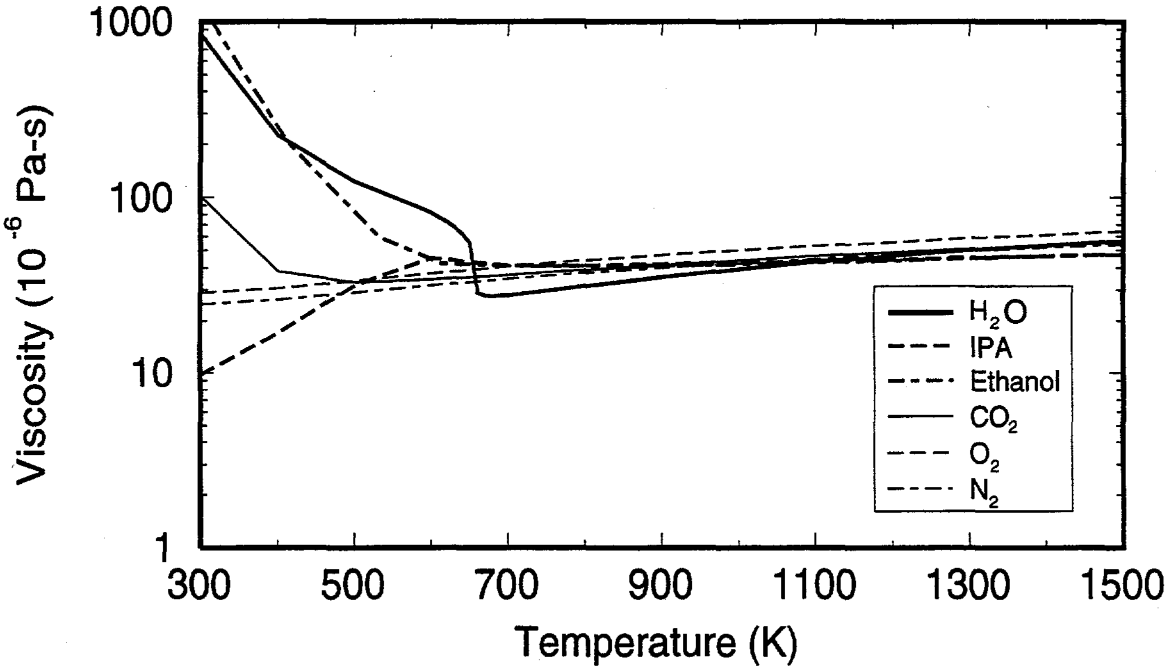

Figure 4. Viscosities of SCWO fluids.

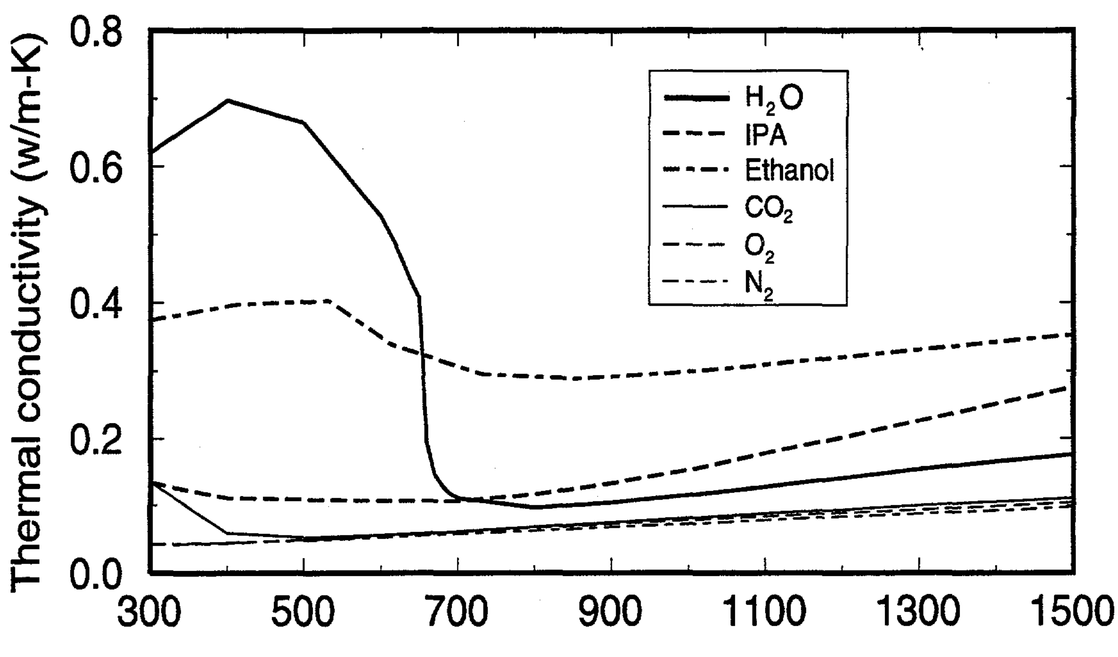

Figure 5. Thermal conductivities of SCWO fluids.

FLUENT computes the mixture density from the individual specie densities as:

$$\rho = \frac{1}{\sum_i \frac{m_i}{\rho_i}}$$

where m_i is the mass fraction and ρ_i is the density of species i.

FLUENT computes the mixture heat capacity, viscosity, and thermal conductivity (shown for heat capacity) as:

$$c_p = \sum_i m_i \, c_{p,i}$$

where $c_{p,i}$ (or μ_i or k_i) are the specie properties.

Figure 6 shows a comparison between the approximations of specific heat of water used in this study and the values predicted using the ASPEN NBS steam tables in Reference 9 . Figure A.37 in Reference 10 shows that the NBS steam tables are very accurate in the vicinity of the critical point .

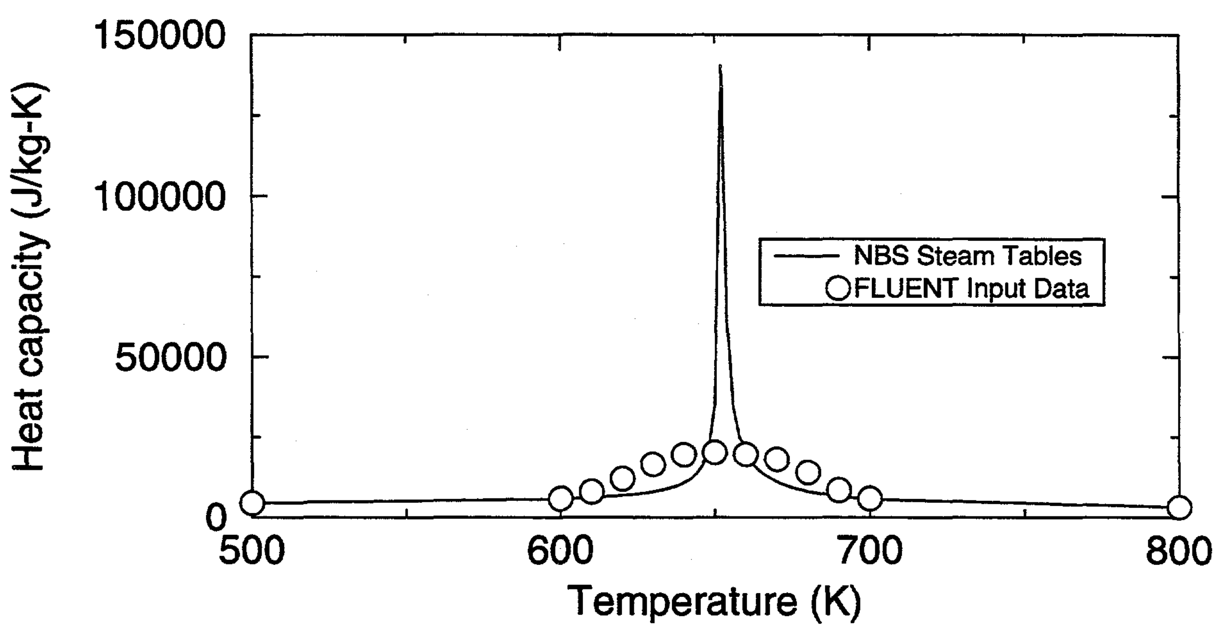

Figure 6. Comparison of water specific heat calculated from NBS steam tables with the approximation used in FLUENT model at 3500 psia and near the critical temperature of 652 K.

4. FLOW SHEET SIMULATION

The SCWO process was simulated using ASPEN PLUS for the baseline and cases replacing CO_2 in the quench stream and a feed stream. The baseline case was based on the MODAR flow sheet with water used in the quench stream. The energy consumption in the baseline is compared with that for CO_2 replacement in the quench stream and a partial replacement in the feed stream.

The mass flow used in this simulation was obtained from MODAR and was scaled up by a factor of 10 because we wanted to evaluate a larger scale than the MODAR's pilot scale.

The basis for and assumptions used in the simulations presented in Section 4 are given below. As additional data are obtained for different equipment or should assumptions regarding operation of the flow sheet be modified, the simulations can easily be rerun.

4.1 Basis for Feeds

4.1.1 Air

2037 lb/hr (467.2 ACFM, 434.4 SCFM), 21 vol% O_2 / 79% N_2 or 23.2 wt% O_2/76.8%N_2.

4.1.2 Water

70^0F from storage tank, 14.7 psia.

Supercritical water - 155 lb/hr (Baseline)
- 2585 lb/hr (Case-A)
- 2869 lb/hr (Case-B)

Quench water (Baseline) - 5950 lb/hr to set the reaction effluent temperature at less than 540^0F.

Water to brine pool - 265 lb/hr.

4.1.3 Simulated Waste

Isopropyl Alcohol - 165 lb/hr, 70^0F, 14.7 psia.

4.1.4 Simulated Impurities

Sodium Chloride - 0.1 lb/hr, 70^0F, 14.7 psia

4.1.5 Pressure profile

The outlet pressure of all high pressure pumps and the air compressor was assumed to be 3600 psia, the outlet of the SCWO reactor 3500 psia, the first stage separator 1500 psia, the second stage separator 100 psia, and the evaporator 14.7 psia.

4.1.6 Air Compressor

The air compressor was simulated as 4-stage compressor with intercoolers on the first three stages only, cooling air to a temperature of 100^0F.

4.1.7 Temperatures

Baseline: Inner nozzle - 100^0F
Outer nozzle - 1112^0F
Case-A: Inner nozzle - 122^0F
Outer nozzle - 930^0F
Case-B: Inner nozzle - 123^0F
Outer nozzle - 1012^0F
Reactor outlet: 1112^0F (600^0C)
Evaporator: 212^0F
Quench stream: < 540^0F

4.1.8 Equation of State Used

The ASME steam table, STEAM-TA, was used for all water streams. The Peng-Robinson cubic equation of state was used for the SCWO reactor and NRTL-RK, also known as the Renon model, for the liquid phase, the Redlich-Kwong equation of state for the gas phase, and Henry's law for supercritical components. The NRTK-RK was used in all the separators where the pressure is much less than that for the reactor.

4.2 Baseline Simulation

The MODAR pilot scale flow sheet is shown in Reference 7 . Stream 1 is air at 70 F and ambient temperature. Air then is compressed at 3598 psia and 475^0F and is combined with water from stream 2. These streams are preheated at B13 and enter the SCWO reactor through the outer nozzle. Stream 3 is isopropyl alcohol (IPA) and is combined with water from stream 2. They enter the SCWO reactor through the inner nozzle. The SCWO reactor is operated at 3500 psia and 1112^0F. B23 is a splitter where the reaction effluents are removed and fed to B32, the brine is mixed with cold water injection from stream 4 and is fed to SEP3, the medium pressure separator via a cooler, B27.

The reaction effluents, CO_2 and water, are quenched with cold water from stream 5 at B32.

MODAR wants to maintain the mixed temperature at less than 572^{0}F (300^{0}C). The quenched stream then is fed through a heat exchanger to reduce the temperature to 100^{0}F before it enters SEP1, the first separator. The first separator is a high pressure separator (1500 psia) to separate the gas and liquid at that condition. Approximately 80% of the CO_2 is removed from this separator via the top, which goes to the atmosphere. Most of the water and remaining CO_2 goes to the second separator, the medium pressure separator, where the remaining CO_2 is removed from the top, and water and residues are separated from the bottom. If the liquid stream contains impurities, e.g., NaCl for this simulation, the impurities are separated at the evaporator. In the MODAR process, the impurities are recycled back to the SCWO feed stream. However, in this study an evaporator was added to remove the impurities and determine the energy consumption.

4.3 CASE-A Simulation

Case-A is a 60% replacement of water by carbon dioxide in the feed stream, and one of the reaction products, carbon dioxide, is recycled to quench the reaction effluent stream.

Since the feed composition to the SCWO reactor is different than in the baseline case, the inlet enthalpy is changed. In order to maintain the reactor temperature at less than 600^{0}C, the inlet stream temperature needs to be calculated. This enthalpy calculation was performed using the enthalpy equation as described in Section 3.

As shown in Figure 8 in Section 5, carbon dioxide, a reaction product, is separated at the first separator, SEP1, and is recycled to quench the hot reaction effluents to 521^{0}F. Before the carbon dioxide is fed to the first separator, the air and carbon dioxide are separated in block B2. The separation unit, B2, could be a membrane separator. Parametric studies on removing carbon dioxide from the air and combustion gases indicate that membrane separation is feasible existing plant technology.

4.4 CASE-B Simulation

The Case-B simulation is very similar to that of the Case-A simulation. The only difference is that Case-B condenses a 20% replacement of water by carbon dioxide in the feed stream vs. 40% for Case-A. The Case-B simulation was performed prior to Case-A. However, it is presented in the later section. The concept of using carbon dioxide in the quench stream is the same as the Case-A.

5. SIMULATION RESULTS

Results for three cases are shown in the following flow sheets, together with tables for each case. The flow sheets show the unit operations with flow rates, temperatures, pressures, heat/ cooler duties and pump horsepower. Stream component and fow rates are given on material balance tables following each flow sheet. The cases shown include the baseline case (no CO_2), Case-A (40% CO_2 in the core feed), and Case-B (20% CO_2 in the core feed).

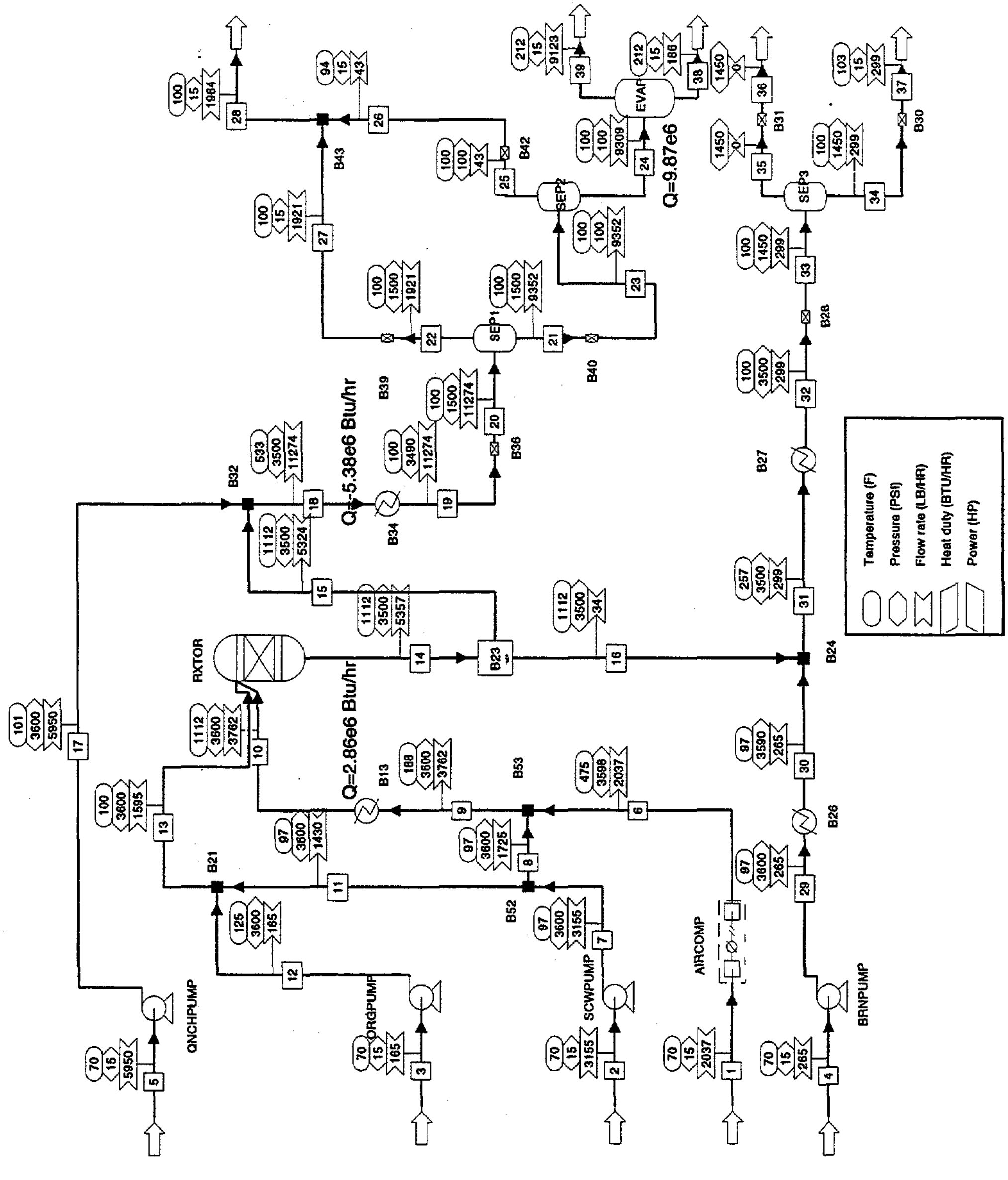

Figure 7. SCWO Flow Sheet for Baseline Case.

MODAR pilot scale run 920													
Stream ID		1	2	3	4	5	6	7	8	9	10	11	12
Temperature	F	70.0	70.0	70.0	70.0	70.0	474.5	96.6	96.6	187.7	1112.0	96.6	125.2
Pressure	PSI	14.70	14.70	14.70	14.70	14.70	3598.00	3600.00	3600.00	3600.00	3600.00	3600.00	3600.00
Vapor Frac		1.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.427	1.000	0.000	0.000
Mole Flow	LBMOL/HR	70.812	175.129	2.747	14.710	330.275	70.812	175.129	95.752	166.564	166.564	79.377	2.747
Mass Flow	LB/HR	2037.000	3155.000	165.100	265.000	5950.000	2037.000	3155.000	1725.000	3762.000	3762.000	1430.000	165.100
Volume Flow	CUFT/HR	27367.639	50.635	3.212	4.253	95.572	213.791	50.317	27.511	175.787	762.788	22.806	3.348
Enthalpy	MMBTU/HR	-0.004	-21.542	-0.358	-1.809	-40.603	0.193	-21.429	-11.716	-11.523	-8.663	-9.712	-0.351
Mass Flow	LB/HR												
O2		428.000					428.000			428.000	428.000		
N2		1609.000					1609.000			1609.000	1609.000		
IPA				165.000									165.000
WATER			3155.000		265.000	5950.000		3155.000	1725.000	1725.000	1725.000	1430.000	
CO2													
NACL				0.100									0.100
Mass Frac													
O2		0.210					0.210			0.114	0.114		
N2		0.790					0.790			0.428	0.428		
IPA				0.999									0.999
WATER			1.000		1.000	1.000		1.000	1.000	0.459	0.459	1.000	
CO2													
NACL				606 PPM									606 PPM

MODAR pilot scale run 920													
Stream ID		13	14	15	16	17	18	19	20	21	22	23	24
Temperature	F	100.3	1112.0	1112.0	1112.0	100.9	532.7	100.0	100.0	100.0	100.0	100.0	100.0
Pressure	PSI	3600.00	3500.00	3500.00	3500.00	3600.00	3500.00	3490.00	1500.00	1500.00	1500.00	100.00	100.00
Vapor Frac		0.000	1.000	1.000	1.000	0.000	0.188	0.109	0.111	0.000	1.000	0.002	0.000
Mole Flow	LBMOL/HR	82.124	252.807	250.946	1.861	330.275	581.221	581.221	581.221	516.521	64.700	516.521	515.381
Mass Flow	LB/HR	1595.100	5357.100	5323.571	33.529	5950.000	11273.571	11273.571	11273.571	9352.322	1921.249	9352.322	9309.240
Volume Flow	CUFT/HR	26.577	1139.452	1131.701	7.621	97.191	500.113	265.031	403.634	152.540	251.094	219.130	151.860
Enthalpy	MMBTU/HR	-10.063	-18.780	-18.600	-0.180	-40.389	-58.989	-64.366	-64.383	-63.249	-1.135	-63.269	-63.149
Mass Flow	LB/HR												
O2			32.647	32.647			32.647	32.647	32.647	0.445	32.202	0.445	0.025
N2			1609.000	1609.000			1609.000	1609.000	1609.000	11.973	1597.027	11.973	0.360
IPA		165.000											
WATER		1430.000	3352.852	3319.323	33.529	5950.000	9269.323	9269.323	9269.323	9267.817	1.506	9267.817	9267.609
CO2			362.501	362.501			362.501	362.501	362.501	71.987	290.515	71.987	41.146
NACL		0.100	0.100	0.100			0.100	0.100	0.100	0.100		0.100	0.100
Mass Frac													
O2			0.006	0.006			0.003	0.003	0.003	48 PPM	0.017	48 PPM	3 PPM
N2			0.300	0.302			0.143	0.143	0.143	0.001	0.831	0.001	39 PPM
IPA		0.103											
WATER		0.896	0.626	0.624	1.000	1.000	0.822	0.822	0.822	0.991	784 PPM	0.991	0.996
CO2			0.068	0.068			0.032	0.032	0.032	0.008	0.151	0.008	0.004
NACL		63 PPM	19 PPM	19 PPM			9 PPM	9 PPM	9 PPM	11 PPM		11 PPM	11 PPM

MODAR pilot scale run 920

Stream ID		25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
Temperature	F	100.0	93.6	100.0	99.9	96.6	96.6	256.6	100.0	100.0	100.0			103.2	212.0	212.0
Pressure	PSI	100.00	14.70	14.70	14.70	3600.00	3590.00	3500.00	3500.00	1450.00	1450.00	1450.00	1450.00	14.70	14.71	14.71
Vapor Frac		1.000	1.000	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000			0.000	0.000	1.000
Mole Flow	LBMOL/HR	1.140	1.140	64.700	65.840	14.710	14.710	16.571	16.571	16.571	16.571	0.000	0.000	16.571	10.308	505.073
Mass Flow	LB/HR	43.083	43.083	1921.249	1964.331	265.000	265.000	298.529	298.529	298.529	298.529	0.000	0.000	298.529	185.764	9123.477
Volume Flow	CUFT/HR	67.270	459.242	26419.379	26877.908	4.226	4.319	5.366	4.874	4.874	4.874	0.000	0.000	4.883	3.239	245690.094
Enthalpy	MMBTU/HR	-0.120	-0.120	-1.115	-1.235	-1.800	-1.800	-1.980	-2.027	-2.028	-2.028			-2.028	-1.241	-52.030
Mass Flow	LB/HR															
O2		0.421	0.421	32.202	32.622										trace	0.025
N2		11.613	11.613	1597.027	1608.640										trace	0.360
IPA																
WATER		0.208	0.208	1.506	1.714	265.000	265.000	298.529	298.529	298.529	298.529			298.529	185.664	9081.945
CO2		30.841	30.841	290.515	321.355										< 0.001	41.146
NACL															0.100	
Mass Frac																
O2		0.010	0.010	0.017	0.017										trace	3 PPM
N2		0.270	0.270	0.831	0.819										trace	39 PPM
IPA																
WATER		0.005	0.005	784 PPM	873 PPM	1.000	1.000	1.000	1.000	1.000	1.000			1.000	0.999	0.995
CO2		0.716	0.716	0.151	0.164										869 PPB	0.005
NACL															538 PPM	

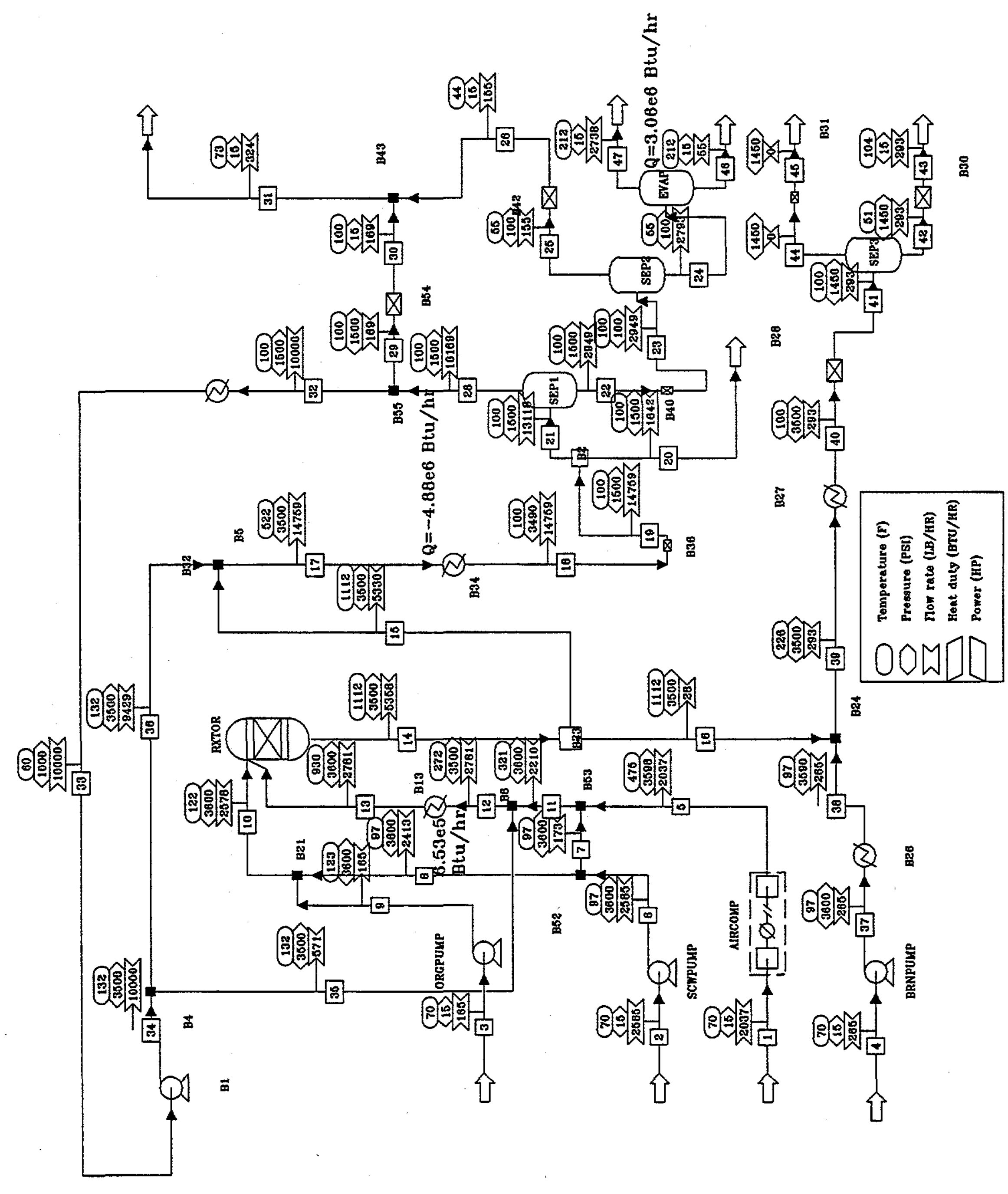

Figure 8. SCWO Flow Sheet for Case-A.

60% SCW and 40% CO2 in the Core Feed													
Stream ID		1	2	3	4	5	6	7	8	9	10	11	12
From						AIRCOMP	SCWPUMP	B52	B52	ORGPUMP	B21	B53	B6
To		AIRCOMP	SCWPUMP	ORGPUMP	BRNPUMP	B53	B52	B53	B21	B21	RXTOR	B6	B13
Phase		VAPOR	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	MIXED
Substream: MIXED													
Mass Flow	LB/HR												
O2		428.0000	0.0	0.0	0.0	428.0000	0.0	0.0	0.0	0.0	0.0	428.0000	428.0000
N2		1609.000	0.0	0.0	0.0	1609.000	0.0	0.0	0.0	0.0	0.0	1609.000	1609.000
IPA		0.0	0.0	165.0000	0.0	0.0	0.0	0.0	0.0	165.0000	165.0000	0.0	0.0
WATER		0.0	2585.000	0.0	265.0000	0.0	2585.000	172.5000	2412.500	0.0	2412.500	172.5000	173.1389
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	570.3611
NACL		0.0	0.0	.1000000	0.0	0.0	0.0	0.0	0.0	.1000000	.1000000	0.0	0.0
Mass Frac													
O2		.2101129	0.0	0.0	0.0	.2101129	0.0	0.0	0.0	0.0	0.0	.1937090	.1539291
N2		.7898871	0.0	0.0	0.0	.7898871	0.0	0.0	0.0	0.0	0.0	.7282190	.5786729
IPA		0.0	0.0	.9993943	0.0	0.0	0.0	0.0	0.0	.9993943	.0640130	0.0	0.0
WATER		0.0	1.000000	0.0	1.000000	0.0	1.000000	1.000000	1.000000	0.0	.9359482	.0780719	.0622689
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	.2051290
NACL		0.0	0.0	6.05694E-4	0.0	0.0	0.0	0.0	0.0	6.05694E-4	3.87958E-5	0.0	0.0
Total Flow	LBMOL/HR	70.81213	143.4893	2.747322	14.70973	70.81213	143.4893	9.575205	133.9141	2.747322	136.6614	80.38734	93.38267
Total Flow	LB/HR	2037.000	2585.000	165.1000	265.0000	2037.000	2585.000	172.5000	2412.500	165.1000	2577.600	2209.500	2780.500
Total Flow	CUFT/HR	27365.46	41.48676	3.212387	4.252995	215.4203	41.22650	2.751091	38.47541	3.342847	43.15127	186.4909	201.9247
Temperature	F	70.00000	70.00000	70.00000	70.00000	474.5000	96.64977	96.64977	96.64977	123.3087	121.5794	321.1481	271.6769
Pressure	PSI	14.70000	14.70000	14.70000	14.70000	3598.000	3600.000	3600.000	3600.000	3600.000	3600.000	3600.000	3500.000
Vapor Frac		1.000000	0.0	0.0	0.0	1.000000	0.0	0.0	0.0	0.0	0.0	.9249574	.9220318
Liquid Frac		0.0	1.000000	1.000000	1.000000	0.0	1.000000	1.000000	1.000000	1.000000	1.000000	.0750426	.0779682
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-52.34120	-1.2301E+5	-1.2958E+5	-1.2301E+5	2723.120	-1.2236E+5	-1.2236E+5	-1.2236E+5	-1.2695E+5	-1.2245E+5	-12175.78	-34534.51
Enthalpy	BTU/LB	-1.819535	-6827.949	-2156.184	-6827.949	94.66370	-6791.935	-6791.935	-6791.935	-2112.522	-6492.209	-442.9865	-1159.836
Enthalpy	BTU/HR	-3706.392	-1.7650E+7	-3.5599E+5	-1.8094E+6	1.92830E+5	-1.7557E+7	-1.1716E+6	-1.6386E+7	-3.4878E+5	-1.6734E+7	-9.7878E+5	-3.2249E+6
Entropy	BTU/LBMOL-R	.8647316	-39.20159	-106.5672	-39.20159	-6.306702	-38.36061	-38.36061	-38.36061	-103.3147	-39.54467	-9.820050	-9.631158
Entropy	BTU/LB-R	.0300606	-2.176019	-1.773316	-2.176019	-.2192396	-2.129338	-2.129338	-2.129338	-1.719193	-2.096613	-.3572789	-.3234610
Density	LBMOL/CUFT	2.58765E-3	3.458677	.8552276	3.458677	.3287162	3.480512	3.480512	3.480512	.8218508	3.167031	.4310523	.4624628
Density	LB/CUFT	.0744368	62.30904	51.39481	62.30904	9.455933	62.70240	62.70240	62.70240	49.38903	59.73405	11.84776	13.76999
Average MW		28.76626	18.01528	60.09489	18.01528	28.76626	18.01528	18.01528	18.01528	60.09489	18.86121	27.48567	29.77533

60% SCW and 40% CO2 in the Core Feed													
Stream ID		13	14	15	16	17	18	19	20	21	21	23	24
From		B13	RXTOR	B23	B23	B32	B34	B36	B2	B2	B2	B40	SEP2
To		RXTOR	B23	B32	B24	B34	B36	B2		SEP1	SEP1	SEP2	EVAP
Phase		VAPOR	MIXED	MIXED	VAPOR	MIXED	MIXED	MIXED	VAPOR	MIXED	MIXED	MIXED	LIQUID
Substream: MIXED													
Mass Flow	LB/HR												
O2		428.0000	32.64689	32.64689	0.0	32.64689	32.64689	32.64689	32.64689	0.0	0.0	0.0	0.0
N2		1609.000	1609.000	1609.000	0.0	1609.000	1609.000	1609.000	1609.000	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		173.1389	2783.491	2755.656	27.83491	2766.206	2766.206	2766.206	0.0	2766.206	2766.206	2754.827	2754.680
CO2		570.3611	932.8625	932.8625	0.0	10351.31	10351.31	10351.31	0.0	10351.31	10351.31	193.7009	38.70785
NACL		0.0	.1000000	.1000000	0.0	.1000000	.1000000	.1000000	0.0	.1000000	.1000000	.0999999	.0999999
Mass Frac													
O2		.1539291	6.09300E-3	6.12482E-3	0.0	2.21196E-3	2.21196E-3	2.21196E-3	.0198866	0.0	0.0	0.0	0.0
N2		.5786729	.3002930	.3018612	0.0	.1090163	.1090163	.1090163	.9801133	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		.0622689	.5194921	.5169829	1.000000	.1874216	.1874216	.1874216	0.0	.2108771	.2108771	.9342742	.9861078
CO2		.2051290	.1741032	.1750124	0.0	.7013434	.7013434	.7013434	0.0	.7891153	.7891153	.0656918	.0138564
NACL		0.0	1.86633E-5	1.87608E-5	0.0	6.77541E-6	6.77541E-6	6.77541E-6	0.0	7.62334E-6	7.62334E-6	3.39141E-5	3.57976E-5
Total Flow	LBMOL/HR	93.38267	234.1625	232.6174	1.545072	447.2111	447.2111	447.2111	58.45689	388.7542	388.7542	157.3192	153.7892
Total Flow	LB/HR	2780.500	5358.100	5330.265	27.83491	14759.26	14759.26	14759.26	1641.647	13117.62	13117.62	2948.628	2793.488
Total Flow	CUFT/HR	412.3832	1102.758	1096.070	6.513201	1144.904	330.6548	749.9670	233.4406	305.7128	305.7128	301.6840	44.37644
Temperature	F	930.0000	1112.000	1112.000	1112.000	522.2615	100.0000	100.0000	100.0000	100.0000	100.0000	100.0000	54.74842
Pressure	PSI	3600.000	3500.000	3500.000	3500.000	3500.000	3490.000	1500.000	1500.000	1500.000	1500.000	100.0000	100.0000
Vapor Frac		1.000000	.9999926	.9999925	1.000000	.9999960	.6593747	.6577915	1.000000	.6078796	.6078796	.0281232	0.0
Liquid Frac		0.0	7.37526E-6	7.42407E-6	0.0	3.99373E-6	.3406253	.3422085	0.0	.3921203	.3921203	.9718767	1.000000
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-27547.80	-75960.30	-75823.02	-96856.50	-1.2238E+5	-1.3329E+5	-1.3230E+5	-96.22086	-1.5327E+5	-1.5327E+5	-1.2453E+5	-1.2350E+5
Enthalpy	BTU/LB	-925.1888	-3319.657	-3308.983	-5376.353	-3708.089	-4038.647	-4008.823	-3.426298	-4542.365	-4542.365	-6644.134	-6799.143
Enthalpy	BTU/HR	-2.5725E+6	-1.7787E+7	-1.7638E+7	-1.4965E+5	-5.4729E+7	-5.9607E+7	-5.9167E+7	-5624.772	-5.9585E+7	-5.9585E+7	-1.9591E+7	-1.8993E+7
Entropy	BTU/LBMOL-R	-2.544060	-7.558775	-7.527457	-13.21076	-8.153911	-22.23990	-19.81704	-9.142892	-23.95824	-23.95824	-38.25907	-39.43335
Entropy	BTU/LB-R	-.0854418	-.3303376	-.3285048	-.7333095	-.2470665	-.6738772	-.6004634	-.3255664	-.7100272	-.7100272	-2.041250	-2.170915
Density	LBMOL/CUFT	.2264463	.2123426	.2122286	.2372216	.3906100	1.352501	.5963076	.2504143	1.271632	1.271632	.5214701	3.465560
Density	LB/CUFT	6.742515	4.858818	4.863070	4.273614	12.89127	44.63647	19.67989	7.032395	42.90831	42.90831	9.773898	62.94979
Average MW		29.77533	22.88197	22.91430	18.01528	33.00291	33.00291	33.00291	28.08304	33.74271	33.74271	18.74297	18.16439

60% SCW and 40% CO2 in the Core Feed												
Stream ID		25	26	28	29	30	31	32	33	34	35	36
From		SEP2	B42	SEP1	B55	B54	B43	B55	B5	B1	B4	B4
To		B42	B43	B55	B54	B43		B5	B1	B4	B6	B32
Phase		VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED												
Mass Flow	LB/HR											
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		.1472212	.1472212	11.37772	.1890785	.1890785	.3362997	11.18864	11.18864	11.18864	.6388716	10.54977
CO2		154.9931	154.9931	10157.61	168.8024	168.8024	323.7954	9988.812	9988.812	9988.812	570.3611	9418.450
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Frac												
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		9.48955E-4	9.48955E-4	1.11886E-3	1.11886E-3	1.11886E-3	1.03754E-3	1.11886E-3	1.11886E-3	1.11886E-3	1.11886E-3	1.11886E-3
CO2		.9990510	.9990510	.9988812	.9988812	.9988812	.9989625	.9988812	.9988812	.9988812	.9988812	.9988812
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow	LBMOL/HR	3.529958	3.529958	231.4350	3.846059	3.846059	7.376016	227.5890	227.5890	227.5890	12.99533	214.5936
Total Flow	LB/HR	155.1403	155.1403	10168.99	168.9914	168.9914	324.1317	10000.00	10000.00	10000.00	571.0000	9429.000
Total Flow	CUFT/HR	187.2278	1288.934	513.0027	8.525237	1563.710	2854.346	504.4774	194.4409	340.2165	19.42636	320.7901
Temperature	F	54.74842	43.90178	100.0000	100.0000	100.0000	73.44510	100.0000	60.00000	131.6183	131.6183	131.6183
Pressure	PSI	100.0000	14.70000	1500.000	1500.000	14.70000	14.70000	1500.000	1000.000	3500.000	3500.000	3500.000
Vapor Frac		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.0	0.0	0.0	0.0
Liquid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-1.6934E+5	-1.6934E+5	-1.7098E+5	-1.7098E+5	-1.6881E+5	-1.6906E+5	-1.7098E+5	-1.7405E+5	-1.7284E+5	-1.7284E+5	-1.7284E+5
Enthalpy	BTU/LB	-3853.011	-3853.011	-3891.371	-3891.371	-3841.962	-3847.250	-3891.371	-3961.166	-3933.706	-3933.706	-3933.706
Enthalpy	BTU/HR	-5.9776E+5	-5.9776E+5	-3.9571E+7	-6.5761E+5	-6.4926E+5	-1.2470E+6	-3.8914E+7	-3.9612E+7	-3.9337E+7	-2.2461E+6	-3.7091E+7
Entropy	BTU/LBMOL-R	-3.631488	.1097627	-10.69097	-10.69097	1.050977	.6129321	-10.69097	-16.18714	-14.74262	-14.74262	-14.74262
Entropy	BTU/LB-R	-.0826284	2.49792E-3	-.2433147	-.2433147	.0239190	.0139480	-.2433147	-.3684014	-.3355258	-.3355258	-.3355258
Density	LBMOL/CUFT	.0188538	2.73867E-3	.4511380	.4511380	2.45957E-3	2.58414E-3	.4511380	1.170479	.6689534	.6689534	.6689534
Density	LB/CUFT	.8286177	.1203633	19.82249	19.82249	.1080708	.1135573	19.82249	51.42951	29.39305	29.39305	29.39305
Average MW		43.94962	43.94962	43.93887	43.93887	43.93887	43.94401	43.93887	43.93887	43.93887	43.93887	43.93887

60% SCW and 40% CO2 in the Core Feed												
Stream ID		37	38	39	40	41	42	43	44	45	46	47
From		BRNPUMP	B26	B24	B27	B28	SEP3	B30	SEP3	B31	EVAP	EVAP
To		B26	B24	B27	B28	SEP3	B30		B31			
Phase		LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MISSING	MISSING	LIQUID	VAPOR
Substream: MIXED												
Mass Flow	LB/HR											
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		265.0000	265.0000	292.8349	292.8349	292.8349	292.8349	292.8349	0.0	0.0	55.38022	2699.300
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.52451E-4	38.70770
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	.0999999	0.0
Mass Frac												
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
WATER		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000			.9981948	.9858628
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			2.74783E-6	.0141371
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0			1.80244E-3	0.0
Total Flow	LBMOL/HR	14.70973	14.70973	16.25481	16.25481	16.25481	16.25481	16.25481	0.0	0.0	3.075764	150.7134
Total Flow	LB/HR	265.0000	265.0000	292.8349	292.8349	292.8349	292.8349	292.8349	0.0	0.0	55.48038	2738.007
Total Flow	CUFT/HR	4.226314	4.318507	5.155236	4.781085	4.781085	4.657605	4.790844	0.0	0.0	.9657269	73049.22
Temperature	F	96.64977	96.60000	225.5032	100.0000	100.0000	51.40759	103.6749			212.0000	212.0000
Pressure	PSI	3600.000	3590.000	3500.000	3500.000	1450.000	1450.000	14.70000	1450.000	1450.000	14.76519	14.76519
Vapor Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	1.000000
Liquid Frac		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000			1.000000	0.0
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
Enthalpy	BTU/LBMOL	-1.2236E+5	-1.2314E+5	-1.2065E+5	-1.2308E+5	-1.2319E+5	-1.2319E+5	-1.2319E+5			-1.2045E+5	-1.0328E+5
Enthalpy	BTU/LB	-6791.935	-6835.546	-6696.845	-6832.148	-6837.843	-6837.843	-6837.843			-6677.884	-5684.867
Enthalpy	BTU/HR	-1.7999E+6	-1.8114E+6	-1.9611E+6	-2.0007E+6	-2.0024E+6	-2.0024E+6	-2.0024E+6			-3.7049E+5	-1.5565E+7
Entropy	BTU/LBMOL-R	-38.36061	-39.48794	-35.43946	-39.36805	-39.31999	-39.68880	-39.15815			-34.88838	-8.677739
Entropy	BTU/LB-R	-2.129338	-2.191914	-1.967189	-2.185259	-2.182591	-2.203063	-2.173608			-1.934181	-.4776655
Density	LBMOL/CUFT	3.480512	3.406209	3.153068	3.399816	3.399816	3.489949	3.392890			3.184942	2.06318E-3
Density	LB/CUFT	62.70240	61.36380	56.80339	61.24863	61.24863	62.87242	61.12386			57.44934	.0374816
Average MW		18.01528	18.01528	18.01528	18.01528	18.01528	18.01528	18.01528			18.03780	18.16698

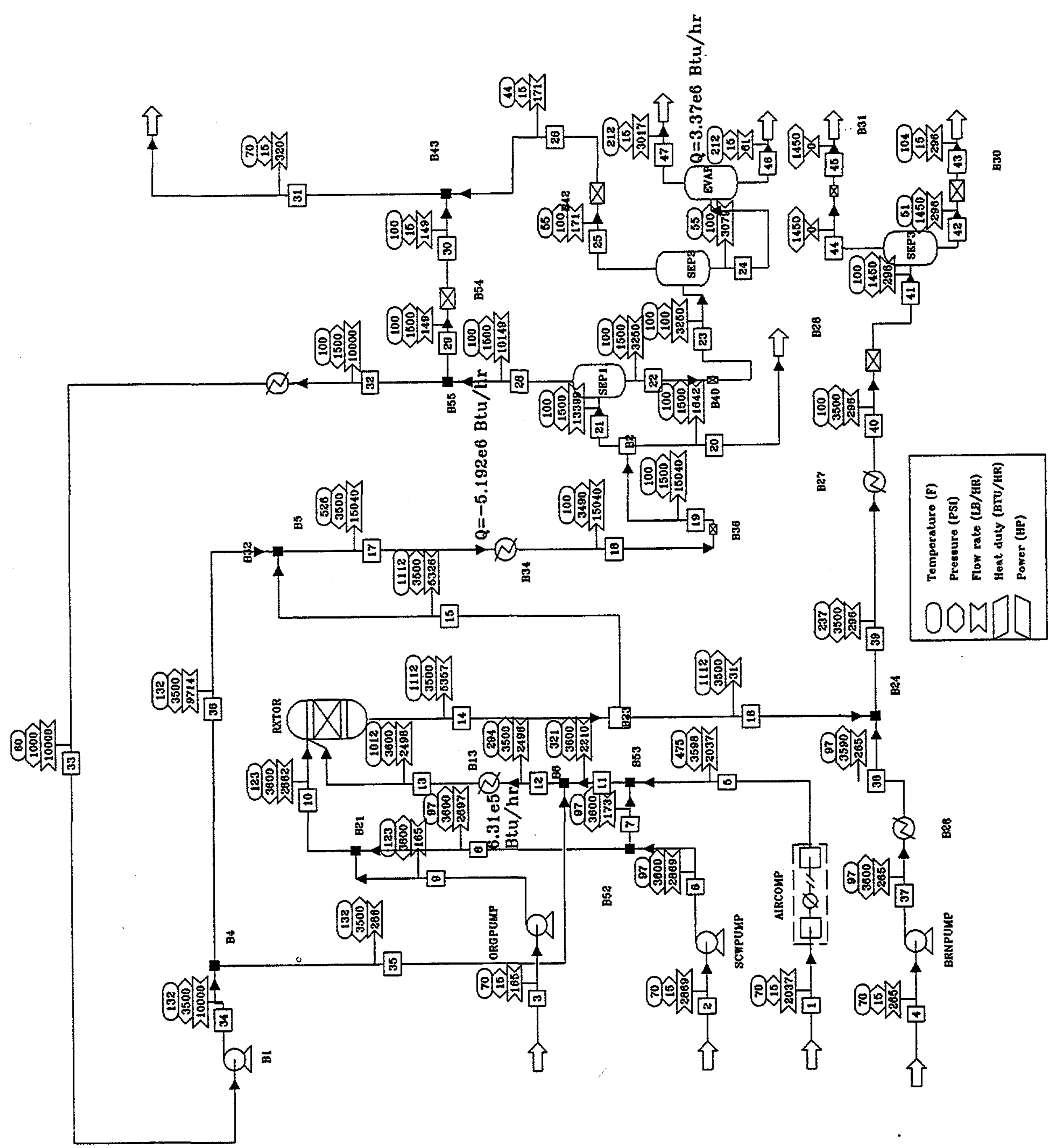

Figure 9. SCWO Flow Sheet for Case-B.

80% SCW and 20% CO2 in the Core Feed													
Stream ID		1	2	3	4	5	6	7	8	9	10	11	12
From						AIRCOMP	SCWPUMP	B52	B52	ORGPUMP	B21	B53	B6
To		AIRCOMP	SCWPUMP	ORGPUMP	BRNPUMP	B53	B52	B53	B21	B21	RXTOR	B6	B13
Phase		VAPOR	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	MIXED
Substream: MIXED													
Mass Flow	LB/HR												
O2		428.0000	0.0	0.0	0.0	428.0000	0.0	0.0	0.0	0.0	0.0	428.0000	428.0000
N2		1609.000	0.0	0.0	0.0	1609.000	0.0	0.0	0.0	0.0	0.0	1609.000	1609.000
IPA		0.0	0.0	165.0000	0.0	0.0	0.0	0.0	0.0	165.0000	165.0000	0.0	0.0
WATER		0.0	2869.000	0.0	265.0000	0.0	2869.000	172.5000	2696.500	0.0	2696.500	172.5000	172.8200
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	285.6800
NACL		0.0	0.0	.1000000	0.0	0.0	0.0	0.0	0.0	.1000000	.1000000	0.0	0.0
Mass Frac													
O2		.2101129	0.0	0.0	0.0	.2101129	0.0	0.0	0.0	0.0	0.0	.1937090	.1715087
N2		.7898871	0.0	0.0	0.0	.7898871	0.0	0.0	0.0	0.0	0.0	.7282190	.6447605
IPA		0.0	0.0	.9993943	0.0	0.0	0.0	0.0	0.0	.9993943	.0576600	0.0	0.0
WATER		0.0	1.000000	0.0	1.000000	0.0	1.000000	1.000000	1.000000	0.0	.9423050	.0780719	.0692526
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	.1144781
NACL		0.0	0.0	6.05694E-4	0.0	0.0	0.0	0.0	0.0	6.05694E-4	3.49455E-5	0.0	0.0
Total Flow	LBMOL/HR	70.81213	159.2537	2.747322	14.70973	70.81213	159.2537	9.575205	149.6785	2.747322	152.4258	80.38734	86.89639
Total Flow	LB/HR	2037.000	2869.000	165.1000	265.0000	2037.000	2869.000	172.5000	2696.500	165.1000	2861.600	2209.500	2495.500
Total Flow	CUFT/HR	27365.46	46.04469	3.212387	4.252995	215.4203	45.75583	2.751091	43.00474	3.342847	47.88659	186.4909	196.7384
Temperature	F	70.00000	70.00000	70.00000	70.00000	474.5000	96.64977	96.64977	96.64977	123.3087	123.0729	321.1481	294.4542
Pressure	PSI	14.70000	14.70000	14.70000	14.70000	3598.000	3600.000	3600.000	3600.000	3600.000	3600.000	3600.000	3500.000
Vapor Frac		1.000000	0.0	0.0	0.0	1.000000	0.0	0.0	0.0	0.0	0.0	.9249574	.9224265
Liquid Frac		0.0	1.000000	1.000000	1.000000	0.0	1.000000	1.000000	1.000000	1.000000	1.000000	.0750426	.0775734
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-52.34120	-1.2301E+5	-1.2958E+5	-1.2301E+5	2723.120	-1.2236E+5	-1.2236E+5	-1.2236E+5	-1.2695E+5	-1.2244E+5	-12175.78	-24210.66
Enthalpy	BTU/LB	-1.819535	-6827.949	-2156.184	-6827.949	94.66370	-6791.935	-6791.935	-6791.935	-2112.522	-6521.956	-442.9865	-843.0450
Enthalpy	BTU/HR	-3706.392	-1.9589E+7	-3.6599E+5	-1.8094E+6	1.92830E+5	-1.9486E+7	-1.1716E+6	-1.8314E+7	-3.4878E+5	-1.8663E+7	-9.7878E+5	-2.1038E+6
Entropy	BTU/LBMOL-R	.8647316	-39.20159	-106.5672	-39.20159	-6.306702	-38.36061	-38.36061	-38.36061	-103.3147	-39.39546	-9.820050	-9.589554
Entropy	BTU/LB-R	.0300606	-2.176019	-1.773316	-2.176019	-.2192396	-2.129338	-2.129338	-2.129338	-1.719193	-2.098436	-.3572789	-.3339201
Density	LBMOL/CUFT	2.58765E-3	3.458677	.8552276	3.458677	.3287162	3.480512	3.480512	3.480512	.8218508	3.183059	.4310523	.4416849
Density	LB/CUFT	.0744368	62.30904	51.39481	62.30904	9.455933	62.70240	62.70240	62.70240	49.38903	59.75787	11.84776	12.68436
Average MW		28.76626	18.01528	60.09489	18.01528	28.76626	18.01528	18.01528	18.01528	60.09489	18.77372	27.48567	28.71811

80% SCW and 20% CO2 in the Core Feed													
Stream ID		13	14	15	16	17	18	19	20	21	22	23	24
From		B13	RXTOR	B23	B23	B32	B34	B36	B2	B2	SEP1	B40	SEP2
To		RXTOR	B23	B32	B24	B34	B36	B2		SEP1	B40	SEP2	EVAP
Phase		VAPOR	MIXED	MIXED	VAPOR	MIXED	MIXED	MIXED	VAPOR	MIXED	LIQUID	MIXED	LIQUID
Substream: MIXED													
Mass Flow	LB/HR												
O2		428.0000	32.64689	32.64689	0.0	32.64689	32.64689	32.64689	32.64689	0.0	0.0	0.0	0.0
N2		1609.000	1609.000	1609.000	0.0	1609.000	1609.000	1609.000	1609.000	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		172.8200	3067.172	3036.500	30.67172	3047.369	3047.369	3047.369	0.0	3047.369	3036.011	3036.011	3035.849
CO2		285.6800	648.1813	648.1813	0.0	10351.31	10351.31	10351.31	0.0	10351.31	213.4715	213.4715	42.65723
NACL		0.0	.1000000	.1000000	0.0	.1000000	.1000000	.1000000	0.0	.1000000	.0999999	.0999999	.0999999
Mass Frac													
O2		.1715087	6.09413E-3	6.12923E-3	0.0	2.17061E-3	2.17061E-3	2.17061E-3	.0198866	0.0	0.0	0.0	0.0
N2		.6447605	.3003491	.3020786	0.0	.1069783	.1069783	.1069783	.9801133	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		.0692526	.5725433	.5700818	1.000000	.2026118	.2026118	.2026118	0.0	.2274363	.9342772	.9342772	.9861115
CO2		.1144781	.1209948	.1216916	0.0	.6882326	.6882326	.6882326	0.0	.7725563	.0656919	.0656919	.0138560
NACL		0.0	1.86668E-5	1.87743E-5	0.0	6.64875E-6	6.64875E-6	6.64875E-6	0.0	7.46337E-6	3.07732E-5	3.07732E-5	3.24822E-5
Total Flow	LBMOL/HR	86.89639	243.4406	241.7381	1.702539	462.8180	462.8180	462.8180	58.45689	404.3611	173.3765	173.3765	169.4862
Total Flow	LB/HR	2495.500	5357.100	5326.428	30.67172	15040.43	15040.43	15040.43	1641.647	13398.78	3249.582	3249.582	3078.606
Total Flow	CUFT/HR	406.5212	1136.785	1129.447	7.176998	1174.517	335.2434	754.5478	233.4406	310.2972	52.38719	332.4761	48.90594
Temperature	F	1012.000	1112.000	1112.000	1112.000	525.8260	100.0000	100.0000	100.0000	100.0000	100.0000	100.0000	54.75034
Pressure	PSI	3600.000	3500.000	3500.000	3500.000	3500.000	3490.000	1500.000	1500.000	1500.000	1500.000	100.0000	100.0000
Vapor Frac		1.000000	.9999929	.9999928	1.000000	.9999961	.6371153	.6355882	1.000000	.5843891	0.0	.0281232	0.0
Liquid Frac		0.0	7.09762E-6	7.14747E-6	0.0	3.86428E-6	.3628847	.3644118	0.0	.4156109	1.000000	.9718768	1.000000
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-16950.47	-75127.06	-74975.40	-96856.50	-1.2172E+5	-1.3294E+5	-1.3200E+5	-96.22086	-1.5211E+5	-1.2390E+5	-1.2453E+5	-1.2350E+5
Enthalpy	BTU/LB	-590.2363	-3413.971	-3402.732	-5376.353	-3745.667	-4090.862	-4061.700	-3.426298	-4590.524	-6610.262	-6644.146	-6799.157
Enthalpy	BTU/HR	-1.4729E+6	-1.8289E+7	-1.8124E+7	-1.6490E+5	-5.6336E+7	-6.1528E+7	-6.1090E+7	-5624.772	-6.1507E+7	-2.1481E+7	-2.1591E+7	-2.0932E+7
Entropy	BTU/LBMOL-R	-2.533908	-8.238831	-8.209482	-13.21078	-8.420218	-22.81701	-20.47440	-9.142892	-24.55066	-37.66201	-38.25909	-39.43336
Entropy	BTU/LB-R	-.0882338	-.3743940	-.3725845	-.7333095	-.2591035	-.7021158	-.6300299	-.3255664	-.7409132	-2.009399	-2.041255	-2.170921
Density	LBMOL/CUFT	.2137561	.2141483	.2140323	.2372216	.3940498	1.380543	.6133713	.2504143	1.303141	3.309520	.5214704	3.465554
Density	LB/CUFT	6.138672	4.712500	4.715963	4.273614	12.80563	44.86421	19.93303	7.032395	43.18047	62.03009	9.773882	62.94953
Average MW		28.71811	22.00578	22.03388	18.01528	32.49750	32.49750	32.49750	28.08304	33.13568	18.74293	18.74293	18.16435

80% SCW and 20% CO2 in the Core Feed												
Stream ID		25	26	28	29	30	31	32	33	34	35	36
From		SEP2	B42	SEP1	B55	B54	B43	B55	B5	B1	B4	B4
To		B42	B43	B55	B54	B43		B5	B1	B4	B6	B32
Phase		VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED												
Mass Flow	LB/HR											
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		.1622605	.1622605	11.35560	.1669377	.1669377	.3291981	11.18867	11.18867	11.18867	.3199958	10.86867
CO2		170.8142	170.8142	10137.85	149.0356	149.0356	319.8498	9988.812	9988.812	9988.812	285.6800	9703.131
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Frac												
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		9.49022E-4	9.49022E-4	1.11887E-3	1.11887E-3	1.11887E-3	1.02817E-3	1.11887E-3	1.11887E-3	1.11887E-3	1.11887E-3	1.11887E-3
CO2		.9990510	.9990510	.9988812	.9988812	.9988812	.9989718	.9988812	.9988812	.9988812	.9988812	.9988812
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow	LBMOL/HR	3.890284	3.890284	230.9846	3.395684	3.395684	7.285968	227.5890	227.5890	227.5890	6.509044	221.0799
Total Flow	LB/HR	170.9765	170.9765	10149.20	149.2025	149.2025	320.1790	10000.00	10000.00	10000.00	286.0000	9714.000
Total Flow	CUFT/HR	206.3403	1420.510	512.0043	7.526929	1380.599	2802.792	504.4774	194.4409	340.2165	9.730192	330.4863
Temperature	F	54.75034	43.90379	100.0000	100.0000	100.0000	70.34032	100.0000	60.00000	131.6183	131.6183	131.6183
Pressure	PSI	100.0000	14.70000	1500.000	1500.000	14.70000	14.70000	1500.000	1000.000	3500.000	3500.000	3500.000
Vapor Frac		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.0	0.0	0.0	0.0
Liquid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	BTU/LBMOL	-1.6934E+5	-1.6934E+5	-1.7098E+5	-1.7098E+5	-1.6881E+5	-1.6909E+5	-1.7098E+5	-1.7405E+5	-1.7284E+5	-1.7284E+5	-1.7284E+5
Enthalpy	BTU/LB	-3853.010	-3853.010	-3891.371	-3891.371	-3841.962	-3847.862	-3891.371	-3961.166	-3933.706	-3933.706	-3933.706
Enthalpy	BTU/HR	-6.5877E+5	-6.5877E+5	-3.9494E+7	-5.8060E+5	-5.7323E+5	-1.2320E+6	-3.8914E+7	-3.9612E+7	-3.9337E+7	-1.1250E+6	-3.8212E+7
Entropy	BTU/LBMOL-R	-3.631454	.1098175	-10.69097	-10.69097	1.050977	.5608596	-10.69097	-16.16714	-14.74262	-14.74262	-14.74262
Entropy	BTU/LB-R	-.0826276	2.49871E-3	-.2433147	-.2433147	.0239190	.0127628	-.2433147	-.3684014	-.3355258	-.3355258	-.3355258
Density	LBMOL/CUFT	.0188537	2.73865E-3	.4511380	.4511380	2.45957E-3	2.59954E-3	.4511380	1.170479	.6689534	.6689534	.6689534
Density	LB/CUFT	.8286141	.1203628	19.82249	19.82249	.1080708	.1142357	19.82249	51.42951	29.39305	29.39305	29.39305
Average MW		43.94962	43.94962	43.93887	43.93887	43.93887	43.94461	43.93887	43.93887	43.93887	43.93887	43.93887

80% SCW and 20% CO2 in the Core Feed												
Stream ID		37	38	39	40	41	42	43	44	45	46	47
From		BRNPUMP	B26	B24	B27	B28	SEP3	B30	SEP3	B31	EVAP	EVAP
To		B26	B24	B27	B28	SEP3	B30		B31			
Phase		LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MISSING	MISSING	LIQUID	VAPOR
Substream: MIXED												
Mass Flow	LB/HR											
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		265.0000	265.0000	295.6717	295.6717	295.6717	295.6717	295.6717	0.0	0.0	61.03592	2974.813
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.68014E-4	42.65706
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	.0999999	0.0
Mass Frac												
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
N2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
IPA		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
WATER		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000			.9983616	.9858633
CO2		0.0	0.0	0.0	0.0	0.0	0.0	0.0			2.74820E-6	.0141367
NACL		0.0	0.0	0.0	0.0	0.0	0.0	0.0			1.63569E-3	0.0
Total Flow	LBMOL/HR	14.70973	14.70973	16.41227	16.41227	16.41227	16.41227	16.41227	0.0	0.0	3.389724	166.0965
Total Flow	LB/HR	265.0000	265.0000	295.6717	295.6717	295.6717	295.6717	295.6717	0.0	0.0	61.13609	3017.470
Total Flow	CUFT/HR	4.226314	4.318507	5.245198	4.827402	4.827402	4.702725	4.837255	0.0	0.0	1.064425	80501.02
Temperature	F	96.64977	96.60000	237.1190	100.0000	100.0000	51.40759	103.6749			212.0000	212.0000
Pressure	PSI	3600.000	3590.000	3500.000	3500.000	1450.000	1450.000	14.70000	1450.000	1450.000	14.76595	14.76595
Vapor Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	1.000000
Liquid Frac		1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000			1.000000	0.0
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
Enthalpy	BTU/LBMOL	-1.2236E+5	-1.2314E+5	-1.2042E+5	-1.2308E+5	-1.2319E+5	-1.2319E+5	-1.2319E+5			-1.2045E+5	-1.0328E+5
Enthalpy	BTU/LB	-6791.935	-6835.546	-6684.176	-6832.148	-6837.843	-6837.843	-6837.843			-6678.570	-5684.868
Enthalpy	BTU/HR	-1.7999E+6	-1.8114E+6	-1.9763E+6	-2.0201E+6	-2.0218E+6	-2.0218E+6	-2.0218E+6			-4.0830E+5	-1.7154E+7
Entropy	BTU/LBMOL-R	-38.36061	-39.48794	-35.10914	-39.36805	-39.31999	-39.68880	-39.15815			-34.89125	-8.677848
Entropy	BTU/LB-R	-2.129338	-2.191914	-1.948853	-2.185259	-2.182591	-2.203063	-2.173608			-1.934564	-.4776717
Density	LBMOL/CUFT	3.480512	3.406209	3.129009	3.399816	3.399816	3.489949	3.392890			3.184557	2.06328E-3
Density	LB/CUFT	62.70240	61.36380	56.36998	61.24863	61.24863	62.87242	61.12386			57.43577	.0374836
Average MW		18.01528	18.01528	18.01528	18.01528	18.01528	18.01528	18.01528			18.03572	18.16697

6. ECONOMIC EVALUATION

An economic evaluation was performed between the Baseline and Case-A. Tables 3 and 4 show the comparison, in terms of the unit equipment cost.

Table 3. Equipment cost for the baseline.

Units	Low Value	High Value
Air compressor (500SCFM)	$30,000	$50,000
SCW pump (8 gpm)	$70,000	$100,000
Organic pump (0.5 gpm)	$35,000	$50,000
Quench pump (1.59 cfm)	$20,000	$30,000
Heater for air/water (1000 kW)	$30,000	$50,000
Reactor vessel with two liners	$200,000	$300,000
Brine pump (4.25 ft^3/hr)	$50,000	$70,000
Brine Heater		
Quench piping	$3,500	$5,000
Feed Heater/Effuent cooler	$2,000	$4,000
Cooldown exchanger	$1,000	$1,000
Letdown valve 1 (2500 psia)	$5,000	$6,000
1st separator (2'OD x 3')	$150,000	$200,000
Letdown valve 2 (1500 psia)	$2,000	$3,000
2nd separator (1.5'OD x 2')	$80,000	$100,000
Offgas collection	$2,000	$3,000
Offgas filters	$2,000	$3,000
Evaporator (9.87e6 Btu/hr)	$20,000	$200,000
Brine cooldown	$2,000	$3,000
Brine letdown valve	$40,000	$50,000
Brine separator	$40,000	$50,000
Total	$746,500	$1,231,000

Table 4. Equipment cost for Case-A

Units	Low value	High value
Air compressor (500 SCFM)	$30,000	$50,000
SCW pump (1cfm)	$70,000	$100,000
Organic pump (0.5 gpm)	$35,000	$50,000
CO_2 pump (6cfm)	$20,000	$30,000
Heater for water/air (189 kW)	$20,000	$30,000
Reactor vessel with two liners	$200,000	$300,000
Brine pump (4.25 ft^3/hr)	$50,000	$70.000
Brine Heater		
Quench piping	$3,500	$5,000
Feed exchanger/effluent cooler	$2,000	$4,000
Cooldown exchanger	$5,000	$7,000
Letdown valve 1 (2500 psia)	$5,000	$6,000
CO_2 separator (1st separator)	$150,000	$200,000
Letdown valve 2 (1500 psia)	$2,000	$3,000
2nd separator	$80,000	$100,000
Letdown valve 3 (100 psia)	$500.00	$1,000
3rd separator	$1,000	$2,000
CO_2 condenser (286e3 Btu/hr)	$5,000	$10,000
O_2 offgas collection	$2,000	$3,000
Offgas filters	$2,000	$3,000
Evaporator (3.06e6 Btu/hr)	$20,000	$200,000
Brine cooldown	$2,000	$3,000
Brine letdown valve	$2,000	$3,000
Total	$757,000	$1,250,000

The equipment for Case-A is only slightly higher than for the baseline unit. Since the Case-A replaces the water used in the quench stream, it saves a significant amount of energy in the end process unit. The flow sheet simulation indicates that the heat duty of the evaporator for the Case-A is 3.06e6 Btu/hr vs. 9.87e6 Btu/hr for the baseline.

This is a difference of about 2000 kW for the pilot scale unit. This is a significant energy savings resulting from the replacement of water by CO_2 for the quenching process.

7. CONCLUSIONS

Supercritical water oxidation (SCWO) shows promise as an economical, environmentally-sound technology for effective decontamination of DOE, diverse industrial, military, and municipal wastes. Several process designs are under development to commercialize the technology, and at least one commercial facility of Eco Waste Technologies, Inc. is presently destroying long-chain alcohols, glycols, and amines in aqueous wastes from chemical plants in Austin, Texas.

SCWO technology can qualify as a totally enclosed treatment facility. That is, the treated effluent can be held in reserve and analyzed prior to release to the environment. If the effluent does not meet the specifications of the relevant regulations it can be recycled to the reactor and treated again. This feature guarantees that no uncontrolled emissions of environmentally damaging compounds will occur during SCWO treatment. Note that this feature stands in contrast with incineration where the effluent is emitted continuously.

A mixed waste treatment system will have effluent requirements determined primarily by environmental regulations and policies. The capability of a process to be known as a "closed system", having a very low release to the environment, no liquid waste and a minimal volume of solid waste will be an important factor in selecting treatment technologies and use in mixed waste treatment. The concept of zero discharge, controllable emissions and acceptance by the public is also very important along with costs and schedule of a mixed waste treatment system that ultimately is built and operated.

In order to make the SCWO technology more viable compared to other technologies, this study focused on energy efficiency to use CO_2 as a replacement of water in the quench stream and also in a feed stream. CO_2 is one of the reaction products and is recycled in the SCWO process. In this study, NaCl was simulated as an impurity in the end unit process, that is an evaporator. The result indicates that case -1, replacement of water by CO_2, reduces the energy duty of evaporator by 6.81e6 Btu/hr based on 5330 lb/hr reaction effluent rate from the reactor.

In addition, the replacement of water in the reactor feed by carbon dioxide would alleviate much of the sticky salt deposit problem because the salts remain in a solid form in the carbon dioxide environment as compared to the water environment due to the lower solubility of salt in carbon dioxide. Also, the higher viscosity of carbon dioxide at the supercritical conditions would minimize the corrosion problem because of the lower mass transfer rate of hetroatoms (e.g.,chlorine, sulphur, etc.) to the wall. If we can prove this phenomena by experiments, it will make SCWO even more advantageous compared to other processes. Due to funding limitations, these comparison could not be included in this study. Because of the many advantages offered by the SCWO relative to other technologies, its development should be continued because research is needed to bridge the gap between the pilot scale and commercialization scale in effectively treating all wastes including the DOE mixed wastes.

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